

일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: **PLEN-1**

발표분야: 기초강연

발표종류: 특별강연, 발표일시: 목 09:30, 좌장: 박승민

TiO₂ Photocatalysis: Present Situation and Future Approaches

Akira Fujishima

Tokyo University of Science, Kanagawa Academy of Science and Technology

The field of photocatalysis can be traced back more than 80 years to early observations of the chalking of titania-based paints and to studies of the darkening of metal oxides in contact with organic compounds in sunlight. During the past 20 years, it has become an extremely well researched field due to practical interest in air and water remediation, self-cleaning surfaces, and self-sterilizing surfaces. During the same period, there has also been a strong effort to use photocatalysis for light-assisted production of hydrogen. The fundamental aspects of photocatalysis on the most studied photocatalyst, titania (TiO₂), are still being actively researched and have recently become quite well understood. The mechanisms by which certain types of organic compounds are decomposed completely to carbon dioxide and water have been delineated. However, certain aspects, such as the photo-induced wetting phenomenon, remain controversial, with some groups maintaining that the effect is a simple one in which organic contaminants are decomposed, while other groups maintain that there are additional effects in which the intrinsic surface properties are modified by light. During the past several years, powerful tools such as surface spectroscopic techniques and scanning probe techniques performed on single crystals in ultrahigh vacuum, and ultrafast pulsed laser spectroscopic techniques have been brought to bear on these problems, and new insights have become possible. Quantum chemical calculations have also provided new insights. New materials have recently been developed based on TiO₂, and the sensitivity to visible light has improved. The new information available is staggering, but we hope to offer an overview of some of the recent highlights, as well as to review some of the origins and indicate some possible new directions.

In this lecture, I will follow the history of TiO₂ photocatalysis, outline the contribution of photocatalysis to a comfortable and safe urban environment, and highlight some important points related to the future development of photocatalysis, including the problem of utilizing visible light and the standardization of photocatalytic systems. I will also introduce our Photocatalysis Museum, which is attached to the

Kanagawa Academy of Science and Technology. In addition, I will present some of our recent studies on novel photocatalyst materials and novel applications of photocatalysis.

References

- [1] A. Fujishima, X. Zhang, D. A. Tryk, Surf. Sci. Rep., 2008, 63, 515-582.
- [2] A. Fujishima, X. Zhang, C. R. Chimie 2006, 9, 750-760.
- [3] A. Fujishima, T. N. Rao, D. A. Tryk, J. Photochem. Photobiol. C: Photochem. Rev. 2000, 1, 1-21.



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발표코드: **AWARD-1**

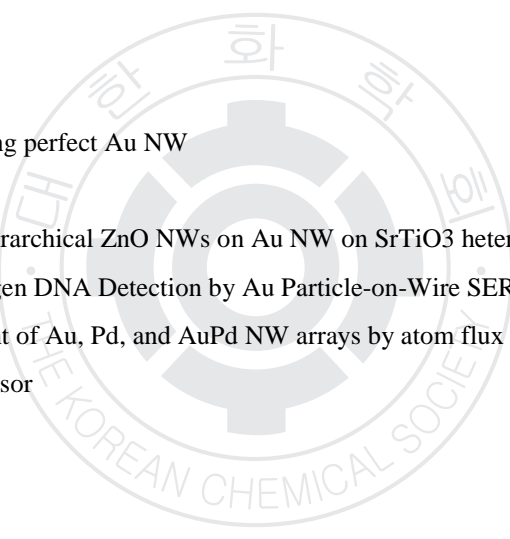
발표분야: 기념강연

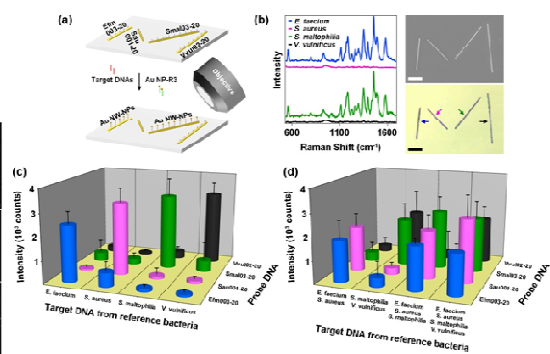
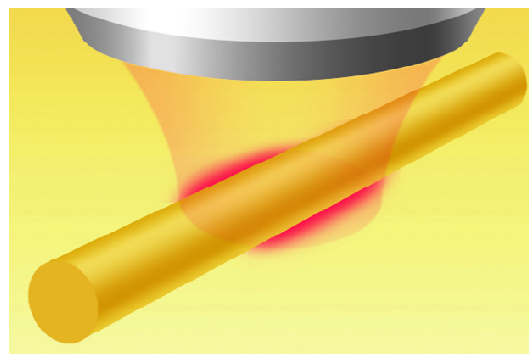
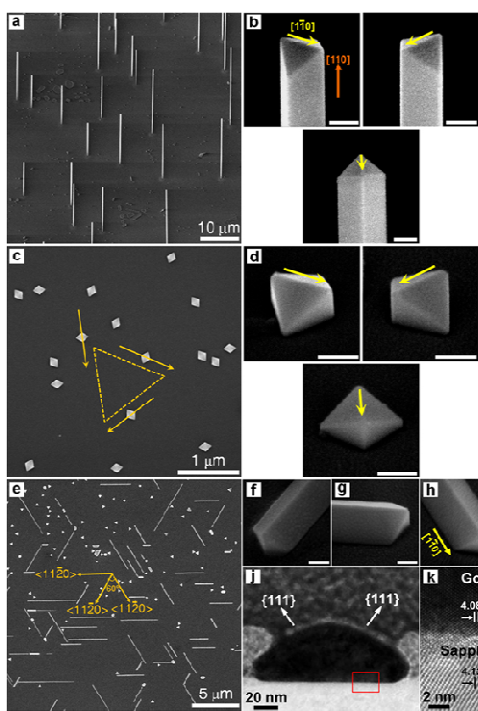
발표종류: 기념강연, 발표일시: 목 11:30, 좌장: 최중길

A Gold Nanowire

김봉수

KAIST 화학과

- 
1. Superelastic Au NW
 2. Superplastic and superstrong perfect Au NW
 3. Rainbow emitting Au NW
 4. Architecturing multiply hierarchical ZnO NWs on Au NW on SrTiO₃ heterostructures
 5. Patterned Multiplex Pathogen DNA Detection by Au Particle-on-Wire SERS Sensor
 6. Steering epitaxial alignment of Au, Pd, and AuPd NW arrays by atom flux change
 7. Au NW-on-Film SERS sensor
 8. Au NW as Nanoelectrode
 9. Au NW as Nanoinjector
 10. Ferromagnetic NWs
 11. In-situ TEM Observation of Heterogeneous Phase Transition of a Constrained Single-crystalline Ag₂Te NW
 12. Diffusion-driven Crystal Structure Transformation: Synthesis of Heusler alloy Fe₃Si NWs



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장소: 제주ICC

발표코드: **POLY1-1**

발표분야: Advanced Materials for Solar Cells

발표종류: 심포지엄, 발표일시: 목 14:00, 좌장: 김범준

Highly efficient polymer solar cells: Processing additives and structures

김진영

울산과학기술대 친환경에너지공학부

Since polymer solar cells continue to be of interest as potential sources of renewable energy, low cost 'plastic' solar cells with high power conversion efficiency (PCE) would have major impact on the needs of our society. By incorporating a few volume percent of alkanedithiols in the solution used to spin cast films comprising a low bandgap polymer and a fullerene derivative, the PCE of photovoltaic cells is increased from 2.8% to 5.5% through altering the bulk heterojunction morphology. We have also fabricated polymer tandem solar cells with a power conversion efficiency of 6.5%, with each layer processed from solution using bulk heterojunction materials comprising semiconducting polymers and fullerene derivatives. Furthermore, inverted polymer solar cells (PSC) with conjugated polyelectrolyte as an electron injection/transporting layer increased the PCE from 2.65 % to 3.55 % by enhancements of the short circuit current and fill factor. The achievement of our PSCs is a major step toward the achievement of high efficiency solar cells that can be fabricated in large areas using low cost printing and coating technologies.

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발표코드: **POLY1-2**

발표분야: Advanced Materials for Solar Cells

발표종류: 심포지엄, 발표일시: 목 14:30, 좌장: 김범준

New Class of Solar Cell Materials: Organic Dyes

김봉수

KIST 태양전지센터

The development of efficient organic solar cells for renewable solar energy conversion has been of great interest as it relates to the worldwide concerns of climate change and energy security. Solar cells based on organic materials have substantial potential for future applications due to the low cost in both materials and device fabrication. Recently, solution-processed bulk heterojunction solar cells based on organic dyes have attracted great attention for their excellent light absorption and stability. When organic dyes are chemically modified with functional groups and/or solubilizing groups to offer optimal optoelectric properties and processibility, we can utilize fully their attractive features (i.e., scalable synthesis, tunable optoelectronic properties through structural control, high carrier mobility, and excellent stability) for organic solar cells. Here we present synthesis and characterization of a new class of solar cell materials based on organic dyes of bodipy and quinacridone.

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발표코드: **POLY1-3**

발표분야: Advanced Materials for Solar Cells

발표종류: 심포지엄, 발표일시: 목 15:30, 좌장: 강영종

Synthesis and Design of Electroactive Polymers for Improving Thermal Stability in Organic Photovoltaics

김범준

KAIST 생명화학공학과

Polymer based organic photovoltaics have attracted a great deal of attention due to the potential cost-effectiveness of light-weight and flexible solar cells. However, most BHJ polymer solar cells are not thermally stable as subsequent exposure to heat drives further development of the morphology towards a state of macrophase separation in the micrometer scale. Here we would like to show three different approaches for developing new electroactive polymers to improve the thermal stability of the BHJ solar cells, which is a critical problem for the commercialization of these solar cells. For one of the examples, we report a new series of functionalized polythiophene (PT-x) copolymers for use in solution processed organic photovoltaics (OPVs). PT-x copolymers were synthesized from two different monomers, where the ratio of the monomers was carefully controlled to achieve a UV photo-crosslinkable layer while leaving the π - π stacking feature of conjugated polymers unchanged. The crosslinking stabilizes PT-x/PCBM blend morphology preventing the macro phase separation between two components, which lead to OPVs with remarkably enhanced thermal stability. The drastic improvement in thermal stabilities is further characterized by microscopy as well as grazing incidence X-ray scattering (GIXS).

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발표코드: **POLY1-4**

발표분야: Advanced Materials for Solar Cells

발표종류: 심포지엄, 발표일시: 목 16:00, 좌장: 강영종

Recent Progress of Electron Accepting Materials for Organic Photovoltaic Cells

윤성철, 이창진

한국화학연구원 화학소재연구단

The power conversion efficiency of Organic Photovoltaic Cells (OPVs) has been remarkably improved from 1% to 8% by development of novel donor and acceptor materials. In the case of acceptors, PCBM has been widely used as electron acceptors for OPVs until the bis-adduct type fullerenes by Plextronics and other researchers. These bis-adducts showed much higher Voc value by modifying the LUMO level of acceptors. During the past 6 years, the authors have also tried to develop the novel acceptor materials such as non-fullerene type acceptors, diketone substituted fullerenes, and self-organizable fullerenes. Recently, novel bis-adduct type fullerenes can be developed in KRICT which show almost similar device performance (5.56% of PCE and 0.81 V of Voc) with Plextronics' acceptor. At this presentation, the progress and status of acceptors for OPVs will be discussed and device performance can be compared by changing the individual acceptor molecules.

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발표코드: **POLY1-5**

발표분야: Advanced Materials for Solar Cells

발표종류: 심포지엄, 발표일시: 목 16:30, 좌장: 강영종

Macroporous structure for energy devices

이현정

국민대 신소재공학부

In this talk, we present a new strategy to fabricate macroporous structures for various energy devices. Macroporous structure provides interconnected paths, which could be electron transport paths in energy devices. Also its large cavities play an important role as scattering voids or spacious room for viscous medium. If it has a periodic and long-range ordered structure, it can modulates a light propagation by a photonic band gap properties. For example, macroporous photoelectrodes having a periodic structured TiO₂ film were fabricated using 2D or 3D polystyrene(PS) microspheres array template. This macroporous structure provides the large surface area leading to the enough adsorption of dye molecules and has a light harvesting effect. Other studies using these macroporous structures will be introduced showing promising potentials for future applications of transparent conductive films, thermoelectric devices and so on as well as solar cells.

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발표코드: **POLY2-1**

발표분야: Young Polymer Chemist Symposium

발표종류: 심포지엄, 발표일시: 금 09:00, 좌장: 박태호

Orthogonal Processing: A New Strategy for Organic Electronics

이진균

인하대 고분자공학과

Organic electronics is an extensively studied subject opening new horizons in electronics technology. It has attracted great attention as a technology to enable flexible devices through solution processing of materials. However, device patterning still remains a hurdle due to problems with chemical processing. Recently, we identified supercritical carbon dioxide and hydrofluoroethers as universal, non-damaging solvents for non-fluorinated materials. These unique solvents expand processing options from the two-dimensional plane to three-dimensional space. Taking advantage of those noble solvents and fluorinated photoresists, we were able to make patterns of functional organic materials down to 5 μm . Furthermore, our orthogonal processing method has been applied to the fabrication of a patterned polymer light-emitting device. In this presentation, a detailed discussion on our orthogonal processing strategy employing scCO₂ and HFEs will be delivered.

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발표코드: **POLY2-2**

발표분야: Young Polymer Chemist Symposium

발표종류: 심포지엄, 발표일시: 금 09:30, 좌장: 박태호

Complex Morphology of ABC Triblock Copolymer

이동현

단국대 고분자시스템공학과

The morphologies in thin films and in the bulk of poly(1,4-isoprene)-block-polystyrene-block-poly(2-vinylpyridine) (IS2VP) were investigated by scanning force microscopy (SFM), transmission electron microscopy (TEM), small angle x-ray scattering (SAXS), grazing incident small angle x-ray scattering (GISAXS) and resonant soft x-ray scattering (RSoXS). In thin films, a hexagonal array of cylindrical microdomains was observed by all methods used, however, with RSoXS, the ability to tune the contrast of the individual components by changing the x-ray energy, showed that the cylindrical microdomains consisted of P2VP cores surrounded by a shell of PS in a PI matrix. In the bulk, SAXS showed a hexagonally packed array of cylindrical microdomains. By selective staining of the blocks, TEM and 3D tomography indicated the presence of two nested arrays of P2VP and PI cylindrical microdomains in a PS matrix. RSoXS unambiguously quantified the co-assembly of two nested hexagonally packed arrays of PI and P2VP cylindrical microdomains in a PS matrix. The cylindrical microdomains of one component were found to be located at the interstitial sites of the hexagonal array of the second component.

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발표코드: **POLY2-3**

발표분야: Young Polymer Chemist Symposium

발표종류: 심포지엄, 발표일시: 금 10:00, 좌장: 박태호

Bioreducible polymers with cell penetrating and endosome buffering functionality for gene delivery systems

김태일

서울대 바이오시스템소재학부

Bioreducible cationic polymers (p(DAH-R/API)s) composed of arginine-grafted diamino-hexane (DAH-R) (cell penetrating functionality) and 1-(3-aminopropyl) imidazole (API) (endosome buffering functionality) monomers were synthesized by Michael reaction of N,N'-cystaminebisacrylamide (CBA) with them, in order to study the effect of endosome buffering moiety on arginine-grafted bioreducible polymeric gene carriers. Several experiments displayed a distinct correlation between monomer composition ratios of p(DAH-R/API)s and the polymer features. Increased endosome buffering capacities proportional to API portions was evaluated for p(DAH-R/API)s due to the imidazole group ($pK_a=6$) of API. Increased portions of API non-ionized at physiological pH and resultant decrease of arginine residues also reduced cytotoxicities of the polymers due to less interaction of cellular compartments with less positively charged polymers, but decreased pDNA condensing abilities, Zeta-potential values, cellular uptakes of polyplexes, and finally transfection efficiencies as well. Thus, the predominance of arginine residues over endosome buffering moieties was revealed regarding efficient gene delivery for p(DAH-R/API)s. From transfection results with chloroquine or nigericin, it can be deduced that the endosomal escape of p(DAH-R/API) polyplexes occurs by direct endosome membrane penetration of arginine moieties as well as endosome buffering abilities of the polymers after cellular uptake, which emphasizes the importance of arginine moieties for polymeric gene delivery systems.

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발표코드: **POLY2-4**

발표분야: Young Polymer Chemist Symposium

발표종류: 심포지엄, 발표일시: 금 10:30, 좌장: 김태일

Hybrid Assemblies of Inorganic Nanoparticles and Amyloid Peptides

유정일

부경대 고분자공학과

The organization of synthetic nanoparticles into one-dimensional (1D) assemblies, such as chains or nanowires, provides a unique pathway to make new materials and realize optoelectronic processes. Similarly, self-organization of natural macromolecules into 1D assembly often plays a crucial role in human health problems. A different parallel can also be made. Similar to the alteration of the optical properties of inorganic nanoparticles that occurs upon assembly, the biological functionality of natural macromolecules can be altered during their self-assembly. In particular, the formation and inhibition of linear chains from amyloid beta-peptides are of great importance because amyloid fibrils are highly implicated in many neurodegenerative diseases, such as Alzheimer's disease. As a matter of fact, some structural, chemical and geometrical characteristics of nanoparticles and natural macromolecules may be quite analogous. From these perspectives, we present (1) the role of CdTe nanoparticles in the process of fibrillation of amyloid peptides (2) the formation of chiral superstructures from CdTe nanoparticles and amyloid fibrils. Kinetic, structural, and conformational ensembles of peptide molecules with CdTe nanoparticles were resolved by experimental and simulation techniques to elucidate a structure-property relationship of the hybrid materials.

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발표코드: **POLY2-5**

발표분야: Young Polymer Chemist Symposium

발표종류: 심포지엄, 발표일시: 금 11:00, 좌장: 김태일

Nanostructured polymers as the building blocks for fabricating state-of-the art sensors

윤현석

전남대 고분자·섬유시스템공학과

There is a growing demand for advanced electronics based on versatile nanomaterials. In this talk, I will discuss i) the synthesis of conducting polymer nanomaterials & their application to electronic sensors and ii) the fluorescent property of single-walled carbon nanotubes (SWNTs) & their application to optical sensors, in which SWNT is functionalized with a water-soluble polymer to make a stable suspension. Conducting polymers are of interest due to the electrical and optical properties that are similar to those of metals or inorganic semiconductors. However, relatively little research has been done on the applications of conducting polymer nanomaterials because of the lack of reliable synthetic methods. In the case of SWNTs, exploration of their optical property remains relatively sparse in the literature while the electrical and mechanical properties have been well studied. These nanomaterials have been successfully employed as transducers to detect various chemical and biological substances.

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발표코드: **POLY2-6**

발표분야: Young Polymer Chemist Symposium

발표종류: 심포지엄, 발표일시: 금 11:30, 좌장: 김태일

고분자 콜로이드의 제조 및 응용

조은철, *정운룡, ** Akira Ohnuma, ***Younan Xia, ****David A. Weitz

한양대 화학공학과 *연세대 신소재공학과 **Hokkaido University, Japan ***Washington University
in St. Louis, U.S.A. ****Harvard University, U.S.A.

본 발표에서는 고분자 콜로이드를 제조하는 일반적인 방법과 최근동향에 대해 문헌을 중심으로 소개할 것이며, 고분자 콜로이드가 어떻게 다양한 분야에 활용되는가에 대해 본인의 연구결과를 중심으로 발표하고자 합니다. 구체적으로 첫째, 온도감응성 hydrogel colloid 의 수용액 상에서 회합거동과 이를 활용한 hydrogel scaffold 의 제조 및 응용에 대해 발표할 예정입니다. 둘째, 고분자 콜로이드기술과 전기방사기술을 활용하여 고분자 콜로이드가 배열된 고분자섬유를 제조하고, 나노섬유 안에 배열된 콜로이드의 특성을 활용하여 두 가지 이상의 약물방출을 제어할 수 있는 가능성에 대해 발표할 예정입니다. 마지막으로 금 나노입자가 포함된 고분자 콜로이드의 제조 방법 및 이에 대한 응용에 대해 발표할 예정입니다.

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장소: 제주ICC

발표코드: **POLY3-1**

발표분야: Carbon-Based Functional Materials

발표종류: 심포지엄, 발표일시: 금 14:00, 좌장: 심상은

Carbon: The Future Materials for Advanced Science and Technology

박수진

인하대 화학과

Carbons have always been the friendliest of materials. Recently, carbon materials are researched as one of promising materials for high-technology fields owing to their increased number of applications including the energy storage devices, aerospace, automotive, rubber, steel, and many other industries. Carbon materials have many advantages due to different allotropes (graphite, diamond, carbon nanotubes, graphene), various textures (micro, meso, and macropore), chemical stability, and endurance from the degree of graphitization or carbonization. In this presentation will cover the state of the art in carbon science and technology and will provide an outlook for the future.

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발표코드: **POLY3-2**

발표분야: Carbon-Based Functional Materials

발표종류: 심포지엄, 발표일시: 금 14:30, 좌장: 심상은

Graphite oxide (and carbon nanotube)/Cellulose Composite using NMMO monohydrate

박수영

경북대 고분자공학과

Graphite oxide (GO)/cellulose composite films were prepared by using a N-methylmorpholine-N-oxide (NMMO) monohydrate solvent. NMMO monohydrate was an excellent dispersing agent for the GO as well as an environmentally friendly solvent for cellulose. The intercalated GO in the cellulose dope was completely exfoliated into the individual carbon layers in the form of graphene oxide by sonication and mechanical stirring. The presence of the small amount of the GO (less than 0.75 wt % of the cellulose) change significantly the rheological properties of the GO/cellulose/NMMO dope, and thermal, electrical, and mechanical properties of the composite films. The viscosity of the GO/cellulose/NMMO dope increased significantly by adding a small amount of the GO in the dope due to the enhanced elastic property through hydrogen bonds between the GO and cellulose. Thermal annealing of the composite films at the relative low temperature (250 °C) removed the oxygen containing groups of the GO in the cellulose matrix and led to improvement of the electrical conductivity of the composite films. More carbonaceous residue was produced by adding a small amount of the GO in the composite after heating in nitrogen atmosphere and might be a positive factor for use as a carbon fiber precursor. The interactions between the GO and cellulose made the composite films strong but brittle by adding a small amount of the GO in the composite.

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발표코드: **POLY3-3**

발표분야: Carbon-Based Functional Materials

발표종류: 심포지엄, 발표일시: 금 15:30, 좌장: 홍창국

Toward Large Scale Separation of Single-Walled Carbon Nanotubes by Electronic Types Using Covalent Functionalization

김우재

경원대 화공환경공학과

The unique structural, electronic, and mechanical properties of single-walled carbon nanotubes (SWNTs) have opened the doors to developments that push the limits of science. These advancements not only further scientific discovery, but also result in the development of everyday practical applications. Certain applications, such as the use of semiconducting SWNTs in transistors and metallic SWNTs in nano-electronic circuits, require the use of SWNTs exhibiting one type of conductivity. However, as-produced SWNTs vary in conductivities, ranging from semiconductors to metals, thus separating and sorting carbon nanotubes, which is a long withstanding problem in the field. This talk will address large volume preparative methods for separating and sorting carbon nanotubes by their electronic structures (metal and semiconductors) and further by their band-gaps (semiconducting SWNTs). Basics of carbon nanotube chemistry will be introduced and how this chemistry is utilized for manipulation of electronic structure of SWNTs and density-induced separation of SWNTs will be discussed. Lastly, recent results of applications of separated SWNTs for high efficient solar funnel and nano-electronic devices will be introduced.

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발표코드: **POLY3-4**

발표분야: Carbon-Based Functional Materials

발표종류: 심포지엄, 발표일시: 금 16:00, 좌장: 홍창국

Hierarchically Assembled Ultrathin Films of Carbon Nanomaterials: Multilayered Opportunity

김병수

울산과학기술대 친환경에너지공학부

Carbon nanomaterials including fullerenes, carbon nanotubes, and graphenes represent the most important class of materials today; their unique physical and chemical attributes advance their roles across most advanced scientific and technology platforms. In this presentation, I will describe our current efforts in developing innovative nanomaterials for energy and biomedical applications based on the carbon nanomaterials, particularly focusing on the layer-by-layer (LbL) self-assembly techniques. LbL assembly has been widely used as a versatile method for fabricating multilayer thin films with controlled structure and composition with a nanometer scale. Due to its facile, inexpensive, and environmentally friendly nature, there have been great interests in utilizing these versatile systems in a number of applications ranging from materials and biological systems. Specifically in this talk, I will illustrate the hierarchical self-assembly of carbon nanomaterials such as multi-walled carbon nanotubes and graphene oxide nanosheets for potential material applications such as transparent conducting thin films, supercapacitors, biosensors, and bioreactors.

일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: POLY3-5

발표분야: Carbon-Based Functional Materials

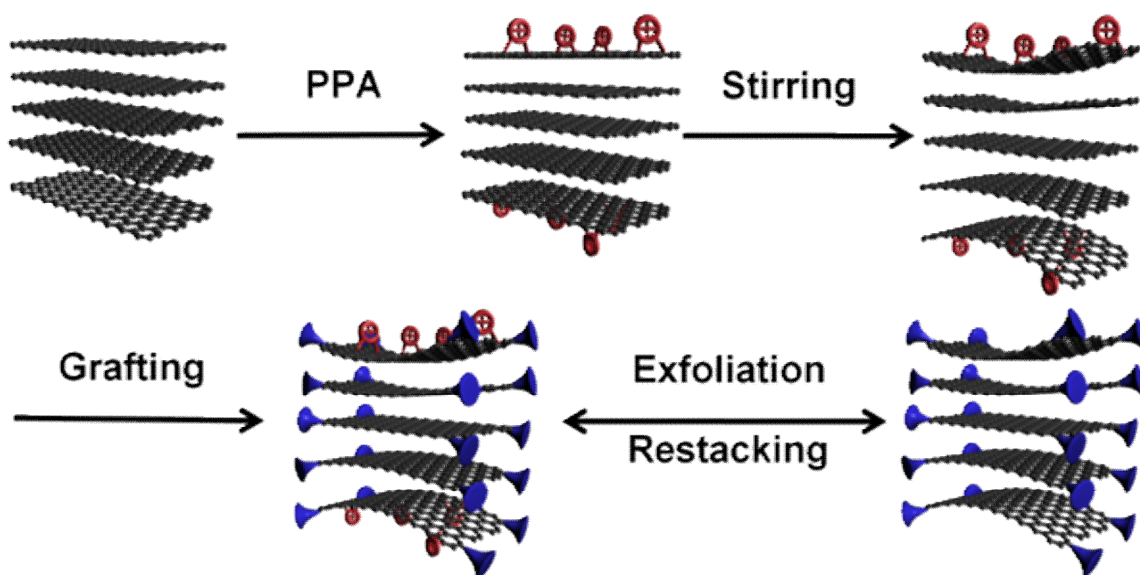
발표종류: 심포지엄, 발표일시: 금 16:30, 좌장: 홍창국

Edge-Functionalized Graphite via Organic Material Wedges: Preparation, Properties, Application

전인엽, 백종범

울산과학기술대 친환경에너지공학부

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. The physical approaches can produce sufficiently to research intrinsic characters of graphene, but their yield is insufficient for practical applications. Hence, chemical approaches draw more attention and have many advantages compared to the physical one. 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) (PPA)/phosphorous pentoxide (P₂O₅) medium. The reaction condition has been previously optimized by functionalization of allotropes of carbon such as carbon nanotubes and carbon nanofibers. This is the first attempt to large-scale “direct” chemical exfoliation of graphite without harsh conditions that are known to damage carbon framework.



일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: IND1-1

발표분야: Hard-coating Materials I

발표종류: 심포지엄, 발표일시: 금 09:00, 좌장: 유복렬

Nanohybrid Silica Based Hard Coating Materials

이종대

조선대 화학과

상업화 되어 있는 대부분의 무기 입자를 함유한 코팅 조성액은 유기바인더를 함께 사용하거나 실란 커플링제를 사용하여 유기 용매에 분산시켜 사용한다. 실란 커플링제로서는 3-(trimethoxysilyl) propylmethacrylate(MPTMS), (3-glycidyloxypropyl)trimethoxysilane (GPTMS), phenyltrimethoxysilane (PTMS), vinyltriethoxysilane (VTES) 등을 사용하며 무기물인 실리카와 유기물의 플라스틱 기관 사이의 접착력을 향상시키는 연구가 활발히 진행중이다. 그러나 유기바인더를 사용할 경우에 유기물의 함량이 늘어남에 따라 표면 경도가 떨어지고, 유기물 함량을 줄이면 분산이 어려워 코팅액으로 사용할 수 없는 단점이 있으며, 실리카와 실란 커플링제의 조성만으로 우수한 표면 경도를 갖는 하드코팅 재료의 제조에는 한계가 있어 왔다. 따라서 이러한 단점들을 해결하기 위하여 본 연구실에서는 나노 입자상태에서 실리카보다 표면 경도가 높은 입자를 졸-겔법으로 제조하여 사용하였고 다양한 실란 커플링제로 표면 개질을 유도하여 유기 용매에 분산성이 우수한 하드 코팅액을 제조하였다. 이러한 코팅 조성은 우수한 표면 경도를 갖는 재료의 특징 때문에 기존 실리카에 비해 내마모성의 향상 특징을 보이며 실란 커플링제로 인한 유기 용매에 우수한 분산성을 갖고 있다. 또한 좀더 높은 표면 경도를 유도하기 위하여 실란 커플링제의 UV 및 열 경화를 유도하여 organic networks 를 형성시켜 보다 높은 표면 경도를 갖는 새로운 하드코팅 재료를 제조할 수 있었다. 이는 다양한 플라스틱 기관과 유리에 우수한 부착성의 특성을 보였다.

일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: IND1-2

발표분야: Hard-coating Materials I

발표종류: 심포지엄, 발표일시: 금 09:30, 좌장: 유복렬

정보소자용 하드코팅재료

강상욱

고려대 소재화학과

다양한 정보소자용 제품 개발에 따라 고기능 하드코팅의 중요성이 그 어느때 보다 증대되고 있다. 일반적으로 PMMA, PET 나 PC 와 같은 투명한 플라스틱 고분자 기판은 광학 장치, 렌즈, 보안경, 디스플레이 장치 등의 분야에서 폭넓게 활용되고 있다. 그러나 표면 경도가 낮고, 마모성에 대한 내구력이 약하며 낮은 내용제성 및 열적 안정성을 갖는 단점이 있다. 또한 김 서림 현상으로 인해 빛의 산란을 유도하여 투명성이 저하되기도 한다. 최근 이러한 단점을 해결하기 위해 다양한 하드코팅 물질들이 개발되고 있으며, 특히 졸-겔법을 이용하여 무기 입자를 포함하고 있는 물질들이 다양한 코팅 산업 분야에 응용되고 있다. 유비쿼터스시대의 정보기기로서 모바일정보 단말기가 확대일로에 있으며, LCD, AMOLED 기반의 모바일 제품에 이르는 다양한 광, 기계적 기능을 요구하고 있다. 또한 정보기기의 휨성 강화에 따른 플라스틱기판의 수요가 기존의 유리 기판을 앞지를 것이라는 판단 하에, 기존의 PC 그리고 PET 미래 수요를 대비한 PEN, TAC 수지를 기저기판으로 한 차세대 정보소자용 하드코팅의 개발현황을 설명한다.

일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: IND1-3

발표분야: Hard-coating Materials I

발표종류: 심포지엄, 발표일시: 금 10:00, 좌장: 유복렬

유-무기 하이브리드 소재를 이용한 기능성 코팅

송기창

건양대 화공생명학과

유-무기 하이브리드 소재는 유기성분과 무기성분이 분자수준 혹은 나노미터 크기로 균일하게 분산되어 있는 소재를 말한다. 졸-겔법은 저온에서 원료용액을 합성하는 공정이므로, 유기성분과 무기성분을 분자수준으로 균일하게 분산시켜 유-무기 하이브리드 코팅용액을 쉽게 제조하는 것이 가능하다. 졸-겔법에 의해 제조된 유-무기 하이브리드 소재의 응용 예로는 하드코팅, 친수성 코팅, 기체 차단성 코팅 등이 있다. 일반적으로 PMMA, PET, PC 와 같은 투명 플라스틱 기재는 가볍고, 내충격성이 강하나 표면경도가 약한 단점이 있다. 이러한 단점을 보완하기 위해 플라스틱 기재 위에 유-무기 하이브리드 소재를 코팅하여 표면경도를 증가시키는데, 이를 하드코팅이라 한다. 본 발표에서는 하드코팅제의 경도 및 굴절률 향상방법, 열경화 및 UV 경화 코팅 기술에 대해 본 연구실에서 연구한 결과를 발표할 예정이다. 또한 플라스틱 기재 위에 유-무기 하이브리드 소재를 코팅하여, 친수성과 기체 차단성 코팅 막을 제조한 내용을 발표하고자 한다.

일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: IND1-4

발표분야: Hard-coating Materials I

발표종류: 심포지엄, 발표일시: 금 10:30, 좌장: 이종대

잉크젯용 고경도·고투명 UV 경화 수지 조성물

김상현

한밭대 응용화학과

본 강의에서는 무기화합물을 함유하는 자외선 경화형 하드 코팅제에 관한 것으로서 투명 플라스틱인 PMMA(polymethylmethacrylate), PET(polyethylene terephthalate), PC(polycarbonate) 같은 투명 플라스틱 및 film 에 피복할 경우 부착성, 내약품성, 내후성 및 내열성등이 향상되며 저장 안정성이 우수한 하드코팅제 제조에 관한 것이다. 이러한 하드코팅제는 고경도·고투명성을 가지는 UV 경화형 하드 코팅제로서 Ink-jetable 의 특성을 가진다. 광경화형 하드코팅제는 각종 디스플레이의 보호용 하드코팅 필름으로서 고경도, 내마모성, 및 내후성이 우수하여 디스플레이의 표면 보호를 위해 매우 적합한 하드코팅에 관한 것이다. 또한 개발된 광경화형 하드코팅제는 잉크젯에 의해 pL(pico-Liter) 단위로 잉크젯 노즐을 통하여 분사 코팅되기 때문에 환경 친화적이며 경제적인 코팅 기술이다.

일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: IND1-5

발표분야: Hard-coating Materials I

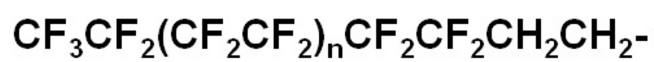
발표종류: 심포지엄, 발표일시: 금 11:00, 좌장: 이종대

Fluorinated materials for hydrophobic and oleophobic coatings

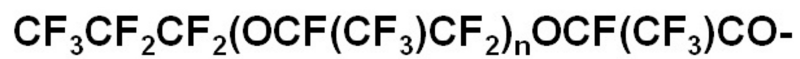
하종욱

한국화학연구원 계면화학공정팀

불소계 고분자 표면개질제는 탄화수소계 고분자에 비해 내열성과 내화학성이 우수하며 매우 낮은 표면에너지를 보이기 때문에 다양한 분야에서 활용되고 있다. 불소계 고분자의 독특한 물성은 불소 원자의 물리화학적 특이성에서 유래되는데 탄소 원자 간의 결합이 인접한 불소 원자에 의해 보호되어, 외부로부터 가해지는 열, 기계 및 화학적 충격에 의한 분해가 쉽지 않다. 또한 불소계 화합물은 일반적인 탄화수소계 물질과 상용성이 좋지 않아 표면 혹은 계면에 배향하거나 각종 매체 내에서 분자결합체를 형성하는 등 표면개질제로서 이상적인 거동을 보이는 것이 알려져 있다. 본 발표에서는 한국화학연구원에서 지난 20 여년 간 수행되었던 불소계 표면개질제의 제조 및 응용에 관한 연구 결과를 요약하여 소개하고자 한다. 첫 번째 주제로서는 섬유 등의 발수발유 가공제로서 오랜 역사를 갖는 과불소알킬 화합물의 제조 및 그 유도체들의 응용에 관한 것으로 과불소알킬알콜의 상업적 제조 공정 개발, 계면활성 및 표면개질 특성에 대한 연구 결과를 소개할 예정이다. 두 번째 주제로서는 최근 본 연구팀에서 집중적으로 수행하고 있는 hexafluoropropylene oxide 의 중합체, 즉 perfluoropolyether 화합물의 합성 및 응용에 관한 연구 결과들을 소개하고자 한다.



(a) perfluoroalkyl compounds



(b) perfluoropolyether compounds



일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: IND1-6

발표분야: Hard-coating Materials I

발표종류: 심포지엄, 발표일시: 금 11:30, 좌장: 이종대

Synthesis and Modification of Monodispersed Spherical Silica

유복렬

KIST 나노재료센터

Silica nanoparticles occupy a prominent position in scientific research, because of their easy preparation and their wide uses in various industrial applications. Many researchers have focused on synthetic approach to get well controlled monodispersed particles and their surface modification with functionalities that can be applicable to composites with organic polymers. In this study, organosilanepolyol was employed as a modifier instead of alkoxysilane. Silica nanoparticles (SNPs) were synthesized by Stöber's method and modified using phenylsilanetriol as a presentative modifier in a range from 0.1 to 10 wt % based on the silica used. The characterizations of all modified particles including particle sizes, surface morphologies, hydrophobicity, etc. were systemically carried out using various analytical tools (SEM, TEM, DLS, BET, etc.). In this seminar, recent results obtained from the surface modification approach to silica and some inorganic oxide particles will be presented in details.

일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: IND2-1

발표분야: Hard-coating Materials II

발표종류: 심포지엄, 발표일시: 금 13:00, 좌장: 김상헌

하드 코팅 재료의 산업적 응용

정희준

(주)디케이씨엠 연구부

산업화 되어 있는 하드 코팅액은 주로 스크린인쇄, Dipping, Spray, Flow coating 법 등을 이용하여 코팅 처리를 한다. 각각의 코팅 처리법에 대하여 코팅액의 기능이 바뀌게 되며, 특히 외관상 점도 변화가 가장 큰 특징이라 할 수 있다. 일반적인 하드 코팅액의 조성은 크게 고분자 수지, 유기 용매, 실리콘 첨가제, 무기 필러 등으로 구성된다. 고분자 수지와 실리콘 첨가제는 코팅액의 부착력, 표면 경도와 관련이 깊으며, 유기 용매는 코팅 처리시 작업성과 유/무기물과의 상용성 및 분산성, 도막의 건조 특성과 연관이 있다. 무기 필러는 소광성, 컬러, 표면 경도 증가의 역할을 하게 된다. 특히 표면 경도와 소광성 증가시키기 위해 실리카를 사용하게 되는데 이는 기재와의 부착력 감소를 초래하므로 새로운 형태의 무기 필러가 필요하게 된다. 특히 기재의 조건에 따른 부착력 변화와 경화 조건에 따른 수지 및 용매의 변화는 User의 다양한 요구에 부합 되어야 하며, 이는 다양한 응용 범위를 갖는 하이브리드 형태의 하드 코팅액 개발의 목표와 일치하게 된다. 본 연구실에서는 실크스크린 인쇄를 통한 하드 코팅액을 개발하여, 멤브레인 스위치와 같은 전극 페이스트 보호용 하드 코팅제에 적용하고 있다.

일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: IND2-2

발표분야: Hard-coating Materials II

발표종류: 심포지엄, 발표일시: 금 13:30, 좌장: 김상헌

Industrial Processing for Hard Coating Materials & Films

장성훈

울촌화학 사업개발팀

광학용 Product 의 고품질 수준을 용이하게 하고, 전후방의 생산 Process 를 용이하게 구축하기 위하여서는 Hard Coating Film Line 을 비롯 PSA(Pressure Sensitive Adhesive), 이형 Film, Solvent Dry Lamination 의 Process 를 Clean Room 환경하에서 일원화하여 운용하여야 하며, Hard Coating 설비에 한해서는 원단의 Anealing, 이물 및 결점의 감지, Web Cleaner, Corona system, 고밀도 제전 System, UV 경화 System 등 Line 의 Process 구조가 필요할 것으로 판단되었다. 이러한 Hard Coating Process 를 통하여 Protection Film 을 합지한 Specialty Film 의 Coating 대응이 가능하고, 특히나 In-line 으로 구성되는 이물 및 검사 Process 를 통해 투과 및 반사를 통한 검사와 Scratch 검사를 운용하여 이물 발생을 사전에 검지함으로써 고수준 품질의 필름 제조를 가능하게 할 것으로 기대되고 있다. 본 기술의 개발을 통해 Anti Finger Print (AFP) Film 을 포함한 Anti Scattering 용 Film, Window Protection film 등 다양한 Hard Coating Film Application 을 구축하는 것이 가능할 것으로 판단된다. Industrial Purpose 를 위한 Key Process 로는 해외에 의존하고 있는 Hard Coating 제에 대한 개발을 병행하는 것이 중요하며 최종 제품의 광학적 물성을 만족하기 위한 기재 Film 의 광학적 특성과 부합한 Hard Coating 제 물성 부여의 검토가 필수적이라고 하겠다.

일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: IND2-3

발표분야: Hard-coating Materials II

발표종류: 심포지엄, 발표일시: 금 14:00, 좌장: 김상헌

정보소자용 하드코팅재료

김현곤

구미전자정보기술원 디스플레이핵심부품국산화지원센터

디스플레이 분야의 디자인 및 기능성이 강조되어감에 따라, 기능성 Polymer 의 중요성도 높아지고 있다. 디스플레이 표시소자에 사용되는 Polymer 는 시인성 및 스크래치 방지를 위해 Polymer 표면에 하드코팅 층을 도포하여 보다 안정성 있는 필름을 구현하고 있다. 현재 개발되고 있는 하드코팅재료는 디스플레이 사용자의 요구에 따라 디스플레이 표면에 지문을 방지하는 내지문 기능성 하드코팅재료를 요구하고 있다. 또한 문자인식 기술의 진화와 함께 손으로 입력을 필요로 하는 터치패널의 경우 인체에서 분비되는 염분, 지방산, 단백질 아미노산등으로 인하여 표시창의 기능을 떨어뜨려 본래의 역할을 달성하지 못한다. 최근 휴대단말의 급속성장으로 터치패널의 탑재가 급속하게 가속됨에 따라 투명패널의 내지문성 부여 기술의 레벨업 요구가 보다 높아져 간다. 내지문성 하드코팅재료를 이용하여 표면의 빛의 반사, 굴절을 막고 표면의 유지 열룩이 남지 않는 불소수지 등의 낮은 표면 에너지를 이용하여 기능성을 부여한 터치패널 하드코팅재료의 개발현황을 설명한다.

일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: IND2-4

발표분야: Hard-coating Materials II

발표종류: 심포지엄, 발표일시: 금 14:30, 좌장: 강상욱

터치패널용 박막코팅소재

윤경근

(주)코오롱 중앙기술원

정전용량방식 터치패널은 애플사의 아이폰을 필두로 하여 스마트폰, 테블릿 PC 의 급격한 확대에 지대한 공헌을 하였으며 앞으로도 디스플레이의 다양한 응용분야를 창출할 것이며 생활 가전에도 접목되어 거대한 트렌드로 자리 매김되어 지고있다. 정전용량 방식 터치패널은 모바일 등 소형에서 점차 그 응용분야가 확대되어 대형화, 슬림화, 플렉서블화로 전개될 전망이다. 이를 현실화하기 위하여 소재의 혁신이 반드시 필요로 하다. 정전용량 방식 터치패널에 사용되는 핵심 소재로 전극이나 배선을 보호하는 고경도, 고내열성의 절연보호막, 굴절율이 조절된 저저항 투명전극용 필름, 고투명 도전성소재, 투명 점착소재, 강화유리대체 기판소재 등이 있다. 사용되는 소재들은 터치패널을 제조하는 공정이나 사용상에 있어 스크래치에 대한 저항성이 있어야 하는데 이를 구현하는 방법에 대하여 알아보겠다.

일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: IND2-5

발표분야: Hard-coating Materials II

발표종류: 심포지엄, 발표일시: 금 15:00, 좌장: 강상욱

전자파차폐용 하드코팅재료

이병섭

(주)지엘켐 영업개발본부

현재 휴대폰,스마트폰,PDA,DMB 등의 모바일 디바이스의 윈도우나 플렉시블 표시소자(Flexible display)기판에 사용되는 기능성 하드코팅액인 경우 수입의 의존도가 높은 것으로 알려져 있다. 이런 이유로 수입에 의존하고 있는 코팅소재의 국산화와 국내원천기술을 확보하는데 의미가 있다본 연구는 실리콘 졸겔공정을 이용한 하드코팅액의 제조방법 및 UV 경화형 수용성 Binder 를 이용하여 전자파차폐용 하드코팅액,코팅막 제조기술을 확보하는데 있으며, 더욱더 구체적으로 CNT, Matel power 와 같은 전자파차폐특성을 나타내는 안료분산액을 제조 및 코팅용 binder 에 첨가하여 기능성 하드코팅액을 제조하고 이것을 플라스틱 기재위에 습도막을 형성한 후 건조과정과 경화공정(열경화, UV curing)을 통하여 기재의 역학적 경도와 차폐성능을 도모하는 하드코팅막의 역할을 갖게 함과 동시에 졸겔 공정을 통한 코팅막을 제조하고 부착성, 표면균질성이 우수한 졸겔코팅막을 형성하여 코팅액과 코팅막의 물성평가를 통하여 코팅액을 개발한다.

일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: IND2-6

발표분야: Hard-coating Materials II

발표종류: 심포지엄, 발표일시: 금 15:30, 좌장: 강상욱

하드코팅과 투명전극

조현남

(주)잉크테크 기술연구소

투명전극 소재는 LCD, PDP, OLED, FED 등의 디스플레이 분야 이외에도 터치패널, 투명 전자파 차폐막, 투명발열체, 도전성 유리, 가스센서, 열반사코팅막, 태양전지, 조명 및 자동차, 투명 정전기 방지막, 통신기기용 안테나, 광학필터 등 초경량, 저전력, 저가격, 휴대성, 고기능성을 특징으로 하는 차세대 플렉시블 디스플레이 및 일렉트로닉스에 응용이 가능한 정보전자 에너지 분야의 핵심 부품 소재이며 여기에는 투명전도 산화물(Transparent conducting oxide, TCO), 탄소나노튜브(CNT), 그래핀(Graphene), 전도성고분자, 은(Ag) 나노와이어(Nanowire) 등 이 잘 알려져 있으며 그 중 디스플레이의 투명전극으로 현재까지 가장 널리 사용되고 있는 ITO(Indium Tin Oxide)는 진공증착 공정과 포토리소그래피 공정에 의해 우수한 전도도와 광투과율, 고밀착성, 고내열성, 표면 평활성 및 가공성 등의 특성을 가지고 있기 때문이다. 따라서 본 심포지움에서는 이러한 투명전극과 하드 코팅의 관계에 관한 논의를 할 것이다.

일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: INOR1-1

발표분야: Inorganic/Material Science in Energy Applications I

발표종류: 심포지엄, 발표일시: 목 14:20, 좌장: 이석중

Dye-sensitized Solar Cells using Metal Substrate

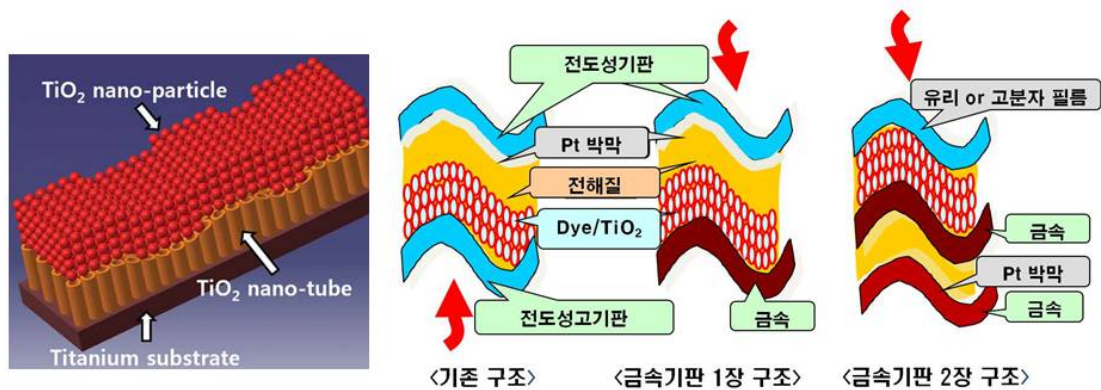
강만구, *정미희, **김점중

한국전자통신연구원 *한국전자통신연구원 박막태양광기술연구팀 **한국전자통신연구원 차세대태양광연구부

반도체 접합 태양전지와는 달리 광합성 원리를 이용한 광전기화학적 염료감응 태양전지는 Grätzel 에 의하여 처음으로 발표된 이후, 10% 이상의 높은 에너지 변환 효율로 많은 관심을 모으고 있으며, 최근 산업계를 중심으로 염료감응 태양전지를 상업화하고자하는 노력이 집중되고 있다. 염료감응 태양전지를 구성하고 있는 소재에서 가격 부담이 큰 전도성기판(F-doped SnO₂ or ITO)을 사용하지 않는 금속기판을 사용한 염료감응 태양전지의 연구결과를 발표하고자 한다. 금속기판을 사용한 염료감응 태양전지는 유연한 플렉서블 태양전지 구현이 가능하여 유비쿼터스 시대의 언제, 어디서나 요구되는 다양한 전원공급이 가능한 보조전원으로 활용가능성이 높을 것으로 예측된다. 본 발표에서는 금속 표면을 화학적 에칭에 의한 표면처리, TiO₂ 나노입자 튜브 코팅 등 금속의 표면 개질에 따른 염료감응 태양전지의 광전기적 특성 변화 결과를 발표하고자 한다. 금속 표면을 최적화하여 9% 이상의 에너지 변환 효율을 얻었으며, 2 장의 금속기판을 사용한 ITO 또는 FTO 전도성기판을 전혀 사용하지 않는 염료감응 태양전지의 구조 및 그 특성을 소개하고자 한다.

참고문헌 1. Ho-Gyeong Yun, Jong Hyeok Park, Byeong-Soo Bae, Man Gu Kang, J. Mater. Chem., Advance Article (DOI: 10.1039/c0jm04210b) (2011)2. Mi-Hee Jung, Man Gu Kang, J. Mater. Chem., Advance Article (DOI: 10.1039/c0jm03431b) (2011)3. Mi-Hee Jung, Ho-Gyeong Yun, Sanghee Kim, Man Gu Kang, Electrochimica Acta, 55 6563–6569 (2010)4. Jong Hyeok Park, Tae-Woo Lee, Man Gu Kang, Chem. Commun., 2867–2869 (2008)5. Yun, H.-G., Jun, Y., Kim, J., Bae, B.-S., Kang, M.G., Applied Physics Letters, 93, 133311 (2008)6. Jong Hyeok Park, Yongseok Jun, Ho-Gyeong Yun, Seung-Yup Lee, and Man Gu Kang, J. Electrochem. Soc. 155, F145-F149 (2008)7. Yongseok Jun and Man Gu Kang, Sol. Energy Mater. Sol. Cells, 91, 779-784 (2007)8. Yongseok Jun and Man Gu Kang, J.

Electrochem. Soc. 154 B68-B71 (2007)9. Man Gu Kang 외 4, Sol. Energy Mater. Sol. Cells, 90, 574-581 (2006)10. Man Gu Kang 외 4, Chem. Lett. 34, 804-805 (2005).



일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: **INOR1-2**

발표분야: Inorganic/Material Science in Energy Applications I

발표종류: 심포지엄, 발표일시: 목 14:55, 좌장: 이석중

Wide Bandgap Inorganic Interlayers for the Polymer Solar Cell

김경곤

KIST 태양전지센터

The active layer of polymer solar cell is based on the bulk heterojunction(BHJ) system. In the BHJ system the electron donating polymer and electron accepting C60 derivatives are blended in one active layer. The blended system causes charge recombination at the interface between the active layer and electrode. To reduce the charge recombination at the interface, it is needed to develop an interlayer that can selectively transfer electrons or holes. We have developed wide band gap inorganic materials for the interlayer of the polymer solar cells. The TiO₂ was used for the electron transporting interlayer and the WO₃ was used for the hole transporting interlayer. We have found that inorganic interlayers enhanced the solar cell efficiency through the reduction of charge recombination at the interface between active layer and electrode. Furthermore, the stability of the polymer solar cell using the interlayer was significantly improved.

일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: **INOR1-3**

발표분야: Inorganic/Material Science in Energy Applications I

발표종류: 심포지엄, 발표일시: 목 15:40, 좌장: 홍창섭

High Efficiency Room Temperature Solid-state Dye-sensitized Solar Cells

장성연

국민대 생명나노화학과

Room temperature solid-state dye sensitized solar cells (DSSCs) fabricated using hierarchically structured TiO₂ as a photoelectrode will be presented. The plastic crystal based solid-state electrolytes were prepared using the succinonitrile as a matrix material. The solid-state DSSCs were fabricated using TiO₂ nanofibers (NF) and nanospheres (NS) that are prepared by electrostatic spinning (e-spin) and spray (e-spray) methods respectively. The resulting TiO₂ photoanode layers using these facile methods contained hierarchical morphology with bimodal pore sizes. The performance of TiO₂-NS and TiO₂-NS based DSSCs were enhanced compared to the DSSCs prepared using the typical TiO₂-NP layers. The power conversion efficiency of the TiO₂-NF and TiO₂-NS based solid-state DSSCs were over 2-fold higher (> 7 %) than that of TiO₂-NP based solid-state DSSCs (~ 3%).

일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: **INOR1-4**

발표분야: Inorganic/Material Science in Energy Applications I

발표종류: 심포지엄, 발표일시: 목 16:15, 좌장: 홍창섭

Recent Progress in Quantum Dots Solar Cells

주진, *김준형

경북대 *경북대 응용화학과

Nanocrystalline particles have attracted broad attention from researchers in various areas for both their fundamental size dependent properties and their many important technological applications. These nanocrystalline materials exhibit size dependent characteristics, and often novel electronic, magnetic, optical, chemical, and mechanical properties that cannot be achieved using their bulk counterparts. Various kinds of nanocrystals have been used for biological labeling and detection, photovoltaic devices, lasers, and catalysis. Among them, this talk will cover the strategies to devise solar cells using quantum dots as an alternative to conventional solar cells. Studies on the synthesis of PbSe quantum dots and brief demonstration will also be presented.

일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: INOR1-5

발표분야: Inorganic/Material Science in Energy Applications I

발표종류: 심포지엄, 발표일시: 목 16:50, 좌장: 홍창섭

Solution-Processable Crystalline Small Molecules for High Performance Photovoltaic Cells

김봉수

KIST 태양전지센터

Progress in organic photovoltaics (OPVs) requires significant advances in the areas of material design and synthesis, film processing, and morphology control, as well as device architecture. One of the most important breakthroughs in OPVs is the introduction of the bulk heterojunction (BHJ) device structure, in which the photoactive thin film consists of a blend of electron donors and acceptors. To date, solution-processed BHJ photovoltaic cells have achieved a power conversion efficiency (PCE) of up to 8%, using various semiconducting polymers as the electron donor and fullerene derivatives as the electron acceptor. In contrast to polymeric systems that intrinsically display large structural variations in molecular weight, polydispersity, and regioregularity, conjugated small molecules and oligomers possess well-defined structures that are relatively easy to modify and purify. In addition, small molecules and oligomers show a strong tendency to self-assemble into ordered crystalline domains with superior charge transport properties and favorable nanoscale phase separation may be achieved via self-assembly of donor and acceptor molecules during solution processing, affording PCEs that have evolved from 1% to 4.4%. Generally, device efficiencies have been limited by issues including poor overlap with the solar spectrum, low molar absorptivity, and low charge mobility. Therefore, the development of new molecular donors with desirable absorption and charge transport properties is important to understand the variables that control the device performance. Here we present our efforts in exploring a series of small molecules for high performance solar cells. Our work demonstrates that solar cell properties are strongly correlated with chemical structures.

일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: INOR2-1

발표분야: Inorganic/Material Science in Energy Applications II

발표종류: 분과기념강연, 발표일시: 금 09:00, 좌장: 나명수

Searching for highly efficient electrode materials for electrochemical energy conversion and storage systems

김민식, 김정호, 양대수, 송민영, 유종성

고려대 신소재화학과

Fuel cells and rechargeable lithium ion batteries are becoming key-enabling technologies and have potential applications in low/zero-emission electric and hybrid vehicles, distributed home power generators, and power sources for small portable electronics. In this study, ordered hierarchical nanostructured carbon (OHNC) with multimodal porosities ranging from macro- to meso-/micropores was investigated as efficient electrode materials in PEMFC and also explored as anode material in Li ion battery. The unique structural characteristics such as large surface area and mesopore volume enable the OHNCs to support high loading Pt nanoparticles with small particle size along with uniform particle dispersion. Pt/OHNCs electrodes have demonstrated considerably improved catalytic activity toward oxygen reduction reaction and markedly enhanced PEMFC polarization performance. In the case of Li ion battery, compared with other porous carbon counterparts such as activated carbon and ordered mesoporous carbon, OHNC also has demonstrated a larger Li ion storage capacity and better rate capability. Such better catalytic activity and capacity performance in fuel cell and Li ion battery are mainly attributable to its fantastic structural characteristics such as large specific surface area and mesoporous volume, particularly well-developed 3D interconnected ordered macropore framework with open mesopores embedded in the macropore walls, facilitating fast mass and charge transport and electron transfer and reducing volume change during the charge-discharge cycling especially at high rates.

일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: **INOR2-2**

발표분야: Inorganic/Material Science in Energy Applications II

발표종류: 심포지엄, 발표일시: 금 09:30, 좌장: 김진홍

가지형 공중합체 기반 고체 염료감응 태양전지 개발

김종학

연세대 화학생명공학과

The morphology of mesoporous TiO_2 films plays an important role in the operation of a DSSC. For example, the energy conversion efficiency of DSSCs with well-organized mesoporous TiO_2 films is much higher than those with traditional films possessing a random morphology. We provide the first report on the successful synthesis of well-organized mesoporous TiO_2 films templated by an organized graft copolymer as a structure directing agent. Well-organized mesoporous TiO_2 films with excellent channel connectivities were developed via the sol gel process using an organized PVC-g-POEM graft copolymer synthesized by one-pot ATRP. The careful adjustment of copolymer composition and solvent affinity using a THF/ H_2O /HCl mixture was used to systematically vary the material structure. We also introduced solid-state polymerizable conductive monomer with good conductivity and penetration to photoelectrode to iodine-free solid-state DSSCs, which involves easily accessible and widely applicable fabrication method. A conducting polymer as a hole transporting material is effectively penetrable into the TiO_2 pores and polymerizable by heating at mild temperatures. The fabricated DSSCs exhibited the highest energy conversion efficiency of 5.4 % in N719 dye.

일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: INOR2-3

발표분야: Inorganic/Material Science in Energy Applications II

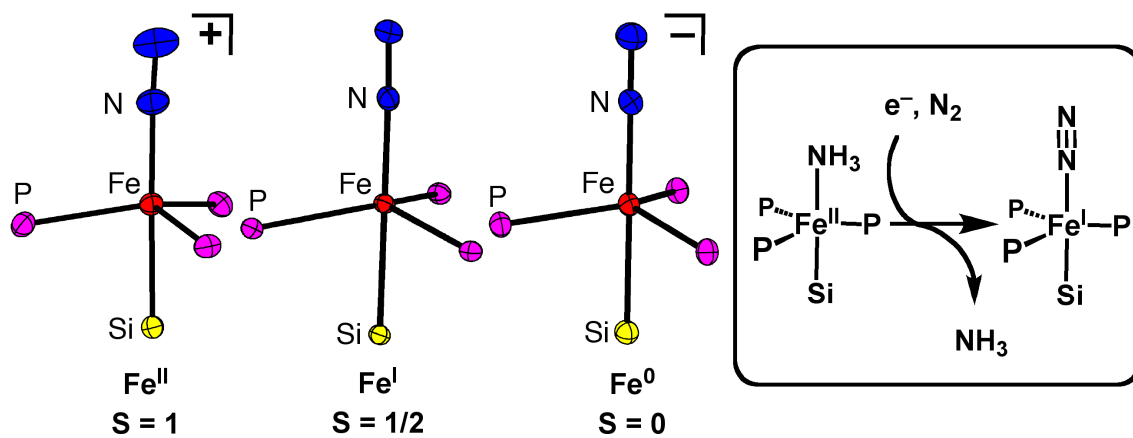
발표종류: 심포지엄, 발표일시: 금 10:00, 좌장: 김진홍

Dinitrogen reduction at the five-coordinate iron center supported by tris(phosphino)silyl ligands

이윤호, *Jonas C. Peters

KAIST 화학과 *California Institute of Technology, Division of Chemistry and Chemical Engineering

Mapping the pathway of dinitrogen reduction by nitrogenase enzymes remains a coveted goal for synthetic chemists. To aid in elucidating the pathways of biological nitrogen fixation, studies of the coordination behavior of various reduced N_2 ligands bound to a single iron site are of interest. The reduction may occur via one of two predominant pathways in which nitrogenous N_xH_y intermediates including hydrazine (N_2H_4), diazene (N_2H_2), nitride (N^{3-}) and imide (NH^{2-}) may be involved. To test the validity of hypotheses concerning iron's direct role in the stepwise reduction of N_2 , iron model systems are needed. Such systems can test the chemical compatibility of iron with various proposed N_xH_y intermediates, and the reactivity patterns of such species. A TBP ($SiPR_3$)Fe-L scaffold ($R = Ph$ and iPr) where the apical site is occupied by nitrogenous ligands such as N_2 , N_2H_4 , NH_3 and N_2R will be described. The system accommodates terminally bound N_2 in the three formal oxidation states (iron(0), +1, and +2). N_2 uptake is demonstrated via displacement of its reduction partners NH_3 and N_2H_4 , and N_2 functionalization is illustrated via electrophilic silylation.



일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: INOR2-4

발표분야: Inorganic/Material Science in Energy Applications II

발표종류: 심포지엄, 발표일시: 금 10:30, 좌장: 김철

Artificial Photosynthesis for Solar Chemicals & Solar Fuel through Photo-bioreactor

백진욱

한국화학연구원 그린화학연구단

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.

일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: INOR2-5

발표분야: Inorganic/Material Science in Energy Applications II

발표종류: 심포지엄, 발표일시: 금 11:00, 좌장: 김철

Titanium Intercalated Layered Double Hydroxides as Highly Efficient Photocatalysts for Water Oxidation under Visible Light

강정구

KAIST 신소재공학과

Selective water oxidation through photocatalytic reaction under visible light irradiation is an important issue in the field of artificial photosynthesis. However, conventional photocatalysts are inefficient when considering the demands of practical application. In this work, we have synthesized a series of titanium intercalated layered double hydroxides (LDH) such as (Ni/Ti)LDH and (Cu/Ti)LDH and tested the compounds for visible light photocatalytic oxygen generation. To demonstrate the photocatalytic ability and the bonding nature of the mixed oxide structures that were prepared in this study, we have characterized them through PXRD, FT-IR, XPS, BET, UV-Vis spectroscopy, TEM and EDX analysis. The intercalation of titanium and the bonding nature of mixed oxide structure of LDHs are proved in this work. The two kinds of LDH show two absorption bands in the visible light area in the red and blue regions that are different from those of pure metal oxide. The more active material between the two LDHs is (Ni/Ti)LDH. The ability of (Ni/Ti)LDH for water oxidation with silver nitrate as sacrificial agent under visible light was found to be 49 μ moles and that of (Cu/Ti)LDH was found to be 31 μ moles under the same conditions

일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: INOR2-6

발표분야: Inorganic/Material Science in Energy Applications II

발표종류: 심포지엄, 발표일시: 금 11:30, 좌장: 김철

Defects in non-photochemical quenching of excessive light energy absorbed by chlorophyll result in the increased production of superoxide from photosystem II in PsbS lacking rice mutant leaves

M. Hall, *윤웅찬, S. Jansson, **이춘환

Umeå University, Sweden *부산대 화학과 **부산대 분자생물학과

Higher plants develop a variety of photoprotective mechanisms against photoinhibition or the light-dependent loss of photosynthetic efficiency. One of the mechanisms against photoinhibition is non-photochemical quenching, especially energy-dependent quenching (qE) of chlorophyll fluorescence. This component depends on three major parameters: the development of transthylakoid proton gradient (ΔpH), the amount of pigments involved in xanthophyll cycle, and the existence of a PsbS subunit in PSII. A rice PsbS T-DNA knock-out line and several RNAi lines were isolated and were deficient in energy-dependent part (qE) of NPQ. The growth rate of young seedlings lacking PsbS was reduced under fluctuating high light condition and photosystem II in detached leaves was more sensitive to photoinhibitory illumination compared to wild-type. Singlet oxygen, superoxide anion radical and hydrogen peroxide levels were determined in leaves histochemically and by fluorescence sensors. PsbS-deficient plants produced more superoxide anion radical and consequently more hydrogen peroxide in chloroplasts and superoxide dismutase activity was increased. The site for superoxide anion radical in PsbS-less plants appeared to be PSII. Genome-wide analysis of the gene expression pattern of the PsbS-KO rice plants shows that lack of PsbS protein led to changes on the transcript level of the 587 genes, presumably as a result of the produced superoxide anion radical in the chloroplast. These data indicate that the specific reactive oxygen species induce specific signaling pathways which activate defense mechanism.

일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: **PHYS1-1**

발표분야: Fundamentals and Applications of Biomaterials

발표종류: 분과기념강연, 발표일시: 목 13:50, 좌장: 신석민

Photodissociation dynamics: multidimensional view

김상규

KAIST 화학과

Here, we present several cases of photodissociation dynamics, where the conical intersection plays an important role along the overall reaction pathway. For reactions on electronically excited states, where transitions occur between adiabatic surfaces, nonadiabatic transitions are essential. The conical intersection where two different adiabatic surfaces touch has been widely accepted as the dynamic funnel for efficient nonadiabatic transitions, and yet the direct experimental probing of the conical intersection has been rare. Here, we investigate the photodissociation of thioanisole and thiophenol, and observe the striking dependence of the reaction product yields on the photoexcitation energy. This results from the unique dynamic process occurring near the conical intersection. The location of the observed resonance on multi-dimensional potential energy surface reveals the nuclear configuration of the conical intersection and its dynamic role in the nonadiabatic transition. Slow electron velocity map imaging method has been employed for the investigation of the predissociation of methylamine on the first excited state. High energy resolved photoelectron images show not only the morphology but also electronic character of the intermediate state which is strongly distorted along the reaction pathway. Preliminary results on the molecular manipulation in the strong electric field will be also briefly introduced.

일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: **PHYS1-2**

발표분야: Fundamentals and Applications of Biomaterials

발표종류: 심포지엄, 발표일시: 목 14:40, 좌장: 장준경

Ultrafast nonlinear optical studies of biomolecular structure and dynamics

조민행

고려대 화학과

Time-resolved vibrational spectroscopy provides direct information on local electrostatic environment, time-dependent conformational changes, and ultrafast chemical exchange dynamics of complex molecules in condensed phases. Over the past decade, two-dimensional (2D) optical spectroscopy has emerged as a promising technique to overcome a number of difficulties associated with conventional linear spectroscopy and has successfully provided intricate details on the structure and dynamics of biomolecules, semiconductor, photosystem, and so on. In particular, the chemical exchange 2DIR spectroscopy, which involves both tagging and probing processes of target vibrational modes with infrared photons, has shown to be an exceptionally useful technique to directly monitor ultrafast chemical or physical processes in condensed phases. Recently, using the chemical exchange 2DIR technique, real time ion-pairing as well as protein dynamics in solutions have been studied. We also have carried out femtosecond IR optical activity measurement by employing a novel spectral interferometry. In parallel with these experimental efforts, we developed time-correlation function theories to directly simulate the vibrational optical activity as well as 2D IR responses of biomolecules in condensed phases using a QM/MM MD simulation method. We anticipate that these novel experimental and computational methods would be of critical use to monitoring molecular motions in real time.

일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: **PHYS1-3**

발표분야: Fundamentals and Applications of Biomaterials

발표종류: 심포지엄, 발표일시: 목 15:05, 좌장: 장준경

Strong positive cooperativity of SNAREs for membrane fusion observed at the single-molecule level

윤태영, *신연균

KAIST 물리학과 *Department of Biochemistry, Biophysics, and Molecular Biology

Single vesicle fluorescence assay detects the fluorescence signals from surface-immobilized nano-scale vesicles. There are three principal labeling positions: vesicle membranes, luminal contents and membrane proteins, each of which allows for study of different aspects of membrane-related biological processes. During the past five years, we have reported two realizations of these possibilities: Measuring the kinetics of single vesicle-vesicle fusion by labeling vesicle membranes and detecting fusion pore opening in such single vesicle fusion by encapsulating fluorescently-labeled DNA hairpins inside vesicles. In this work, by using fluorescently labeled SNARE proteins, we report on the kinetics of SNARE complex formation observed at the single-molecule level. We have developed an advanced single-molecule FRET technique, in which we track not one, but up to 10 proteins at the same time while keeping the precision at the single-molecule level. The measured kinetics of SNARE complex formation shows strong, positive cooperativity. We finally discuss whether we can make two single-molecule measurements in one experimental setting, i.e., detecting the moment of fusion pore opening while tracking formation of multiple SNARE complexes. Such experiment would reveal quantitative correlation between multimeric structure of SNARE proteins and its functional effect on fusion pore opening.

일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: **PHYS1-4**

발표분야: Fundamentals and Applications of Biomaterials

발표종류: 심포지엄, 발표일시: 목 15:30, 좌장: 장준경

Understanding Protein-Protein Interactions in water

합시현

숙명여대 화학과

A number of human diseases, known as amyloid diseases, are associated with the deposition of a variety of insoluble protein aggregates. Under pathological conditions, incorrectly or partially folded proteins can self-assemble by protein-protein interactions (PPIs) into a variety of neurotoxic aggregate species, ranging from soluble oligomers to amyloid fibrils. Understanding the driving factors and mechanistic information of protein aggregation process by PPIs would therefore be necessary in the developments of related therapeutics and medical treatments. Here, I present the atomic-level description for structural and thermodynamic features of PPIs toward protein aggregation related to amyloid disease by using a combined method of molecular simulations and statistical mechanics.

일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: **PHYS1-5**

발표분야: Fundamentals and Applications of Biomaterials

발표종류: 심포지엄, 발표일시: 목 16:10, 좌장: 이연

Mass spectrometry gas-phase approach for the measurement of Zn²⁺ binding constants of Zinc-finger peptides and its noncovalent interactions with DNAs

오한빈

서강대 화학과

Since the advent of soft ionization methods such as electrospray ionization (ESI) and matrix assisted laser desorption/ionization mass spectrometry (MALDI), mass spectrometry has been used for characterization of biomolecules in solution. However, it has been under hot debate whether mass spectral observations genuinely reflects the properties of biomolecules in solution. Among many properties of biomolecules, noncovalent interactions has been an central issue. Recently, our laboratory has studied noncovalent interactions of zinc finger proteins which have substantial potential as a DNA binding motif. First, we've sought to develop a new mass spectrometry method with which we can measure the metal binding constant for zinc fingers. Second, we've studied noncovalent interactions of zinc fingers and DNAs. Many experimental findings suggested that when zinc fingers are involved in the formation of noncovalent complexes with DNAs, its noncovalent complexes observed in ESI-mass spectrum reflect its binding properties with DNAs as in solution. In the symposium, detailed experimental findings will be presented along with its interpretations based on biochemistry in solution. This work is financially supported by the National Research Foundation of Korea (NRF-2009-0075245).

일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: **PHYS1-6**

발표분야: Fundamentals and Applications of Biomaterials

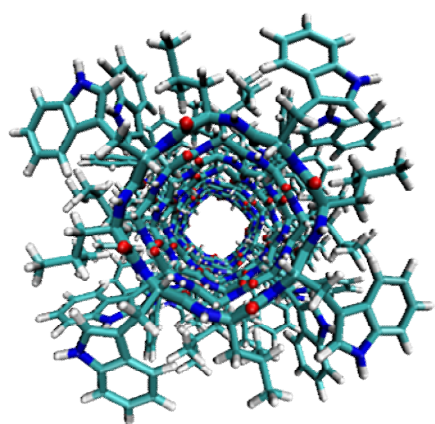
발표종류: 심포지엄, 발표일시: 목 16:35, 좌장: 이연

Potential of mean force calculations of transport of ions and small molecules through a synthetic ion channel

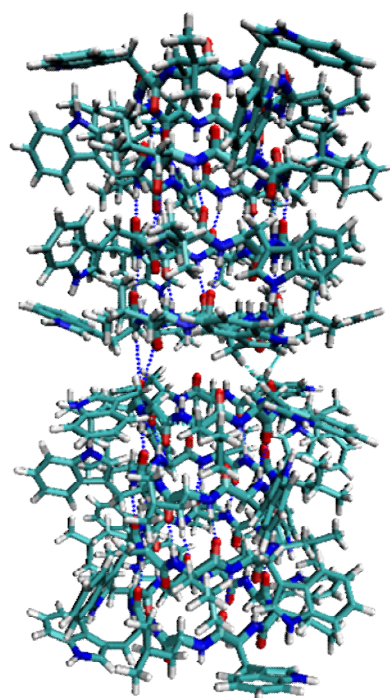
황현석

강원대 화학과

Cyclic peptide nanotubes, a synthetic ion channel, possess similar properties to natural ion channels. Cyclic peptide nanotubes have been considered as an anti-bacterial drug thanks to their relatively simple structure. They can also operate as biosensors to detect ions or small biomolecules due to their selectivity and sensitivity to charges and sizes. In this talk, I present potential of mean force (PMF) calculations to study the transport of ions and small biomolecules through cyclic peptide nanotubes. Molecular dynamics (MD) simulations along with the umbrella sampling method are employed to obtain PMF for ions and small molecules. The ion selectivity and small molecule permeability of cyclic peptide nanotubes are elucidated in terms of PMF calculations. Several issues in the PMF calculation are also addressed.



(a)



(b)



일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: **PHYS1-7**

발표분야: Fundamentals and Applications of Biomaterials

발표종류: 심포지엄, 발표일시: 목 17:00, 좌장: 이연

Dynamic modulation of cell-cell communication by microscope projection photolithography based on a bio-friendly photoresist

도준상

포항공과대 융합생명공학부

Many biological processes in multi-cellular organisms are regulated by dynamic cell-cell interactions. However, classical tissue culture system can only provide static environments where many cell-cell communications occur randomly, thus mechanistic study of dynamics of cell-cell interactions has been limited. To overcome this limitation, we developed a new experimental platform where we can precisely position different types of cells and trigger their interactions by either adding chemicals or irradiating light to certain areas. A thin film of a bio-friendly photoresist PDMP (poly(2,2-dimethoxy nitrobenzyl methacrylate-r-methyl methacrylate-r-poly(ethylene glycol) methacrylate) was used. Upon UV exposure, PDMP thin films become soluble in near-neutral aqueous buffers such as PBS and tissue culture media with minimal cytotoxicity. To create micro-patterns on PDMP thin film, microscope projection photolithography (MPP) technique was used. By performing serious of MPP on PDMP thin films and sequentially depositing proteins and cells on UV-irradiated regions, we could successfully create single cell arrays of adhering cells and pair cell arrays of non-adhering immune cells. Cell-cell communication was initiated by removing PDMP thin films between adhering cells in single cell arrays or by adding antigenic peptide to pair cell arrays of immune cells. Initial stage of cell-cell communication was observed by fluorescence microscopy and interference reflection microscopy. In this way, we could obtain high-resolution view of the onset of cell-cell communication with high-throughput manners.

일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: **PHYS2-1**

발표분야: Computational Chemistry for Energy Materials

발표종류: 심포지엄, 발표일시: 금 09:10, 좌장: 정유성

Computational Materials Design for Molecular Hydrogen Storage

임지순

서울대 물리천문학부

수소는 이산화탄소를 배출하지 않는 차세대 에너지원 중의 하나로 주목받고 있다. 그러나 수소를 연료로 쓸 경우 부피가 엄청나게 커진다는 결점을 극복하고 높은 밀도로 안전하게 저장하는 것이 해결해야 할 큰 과제이다. metal hydride 혹은 chemical hydride 에서 수소가 원자로 분해되어 저장되는 반면 나노구조체에서는 분자형태의 수소를 그 다공성 골격구조에 비교적 약한 결합으로 직접 저장하는 것이 목표이다. 나노다공성 물질에 대한 그 동안의 여러 시도를 간단히 소개하고 아직 괄목할 만한 성공을 거두지 못하고 있는 원인을 분석해 보았다. 전이 금속 원자를 Metal Organic Framework (MOF) 와 같은 골격구조에 부착시켜 Kubas interaction 을 통해 수소분자 저장능력을 향상시키는 computer simulation 결과를 소개하고 실제 공동연구 중인 실험 그룹에서의 진전 상황도 알아본다. 수소분자가 전이금속 원자에 부착되는 결합 에너지가 전자의 스핀상태에 의존함을 규명하고, Ti, Fe 등 유력한 전이금속에 대한 저장능력 계산 결과를 제시하고자 한다. 또한 금속원자들 사이의 cluster 형성을 방지하고 산화를 억제하는 방안에 대해서도 제일원리적 전자구조 계산을 통해 그 가능성을 모색한다. 또한 기존의 MOF 실험 data 를 더 체계적으로 정밀하게 해석할 수 있는 공식을 소개하고 이용할 것이다.

일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: **PHYS2-2**

발표분야: Computational Chemistry for Energy Materials

발표종류: 심포지엄, 발표일시: 금 09:35, 좌장: 정유성

Computational studies on hydrogen storage, organic semiconductor, and explosives

이진용

성균관대 화학과

Hydrogen storage materials have received an intensive spot-light. We proposed a possible way to enhance the hydrogen storage capacity by injecting electrons into the inorganic materials, lithium aluminum hydride (LAH). It was found that when the hydrogen was inserted into the LAH cluster the volume was decreased as an excess electron was added, which enhances the hydrogen storage capacity. As the second example, we will discuss the electron and hole mobility changes of the stacked annelated trithiophenes under the influence of electric field. It was implicated the compound could be n- or p-type depending on the field strength. We adapted p-stacked geometry, while in the previous experiment, the herringbone type was reported. It implies that the geometry could control the p or n-type semiconductor. Finally, we will discuss a new multi-cyclic compound theoretically predicted by stilbene dimer depending on the inter-molecular distance, which would be a possible candidate for explosives.

일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: **PHYS2-3**

발표분야: Computational Chemistry for Energy Materials

발표종류: 심포지엄, 발표일시: 금 10:00, 좌장: 정유성

Joining experimental and theoretical studies of π -conjugated polymers and polymer:fullerene blend

김동욱

경기대 화학과

Organic electronics using polymer materials such as organic photovoltaics (OPVs) have attracted a great deal of interests because they have a variety of potential i.e., their cheap and easy fabrication, possibilities for flexible and/or transparent devices and for large-area devices, etc. The reports have it that devices with power conversion efficiency higher than 7 % have recently been made.¹⁻⁴ In spite of those successful achievements, very little is known as to how these materials pack at the molecular level, although the morphology of polymer films is known to play a critical role on the performance of such devices. This is partly because polymer films usually exhibit amorphous structures, but even for crystalline materials, the thinness of the film and their poly-crystallinity make the experimental analyses at the molecular level difficult. Hence, as a complement to the experiments, theoretical simulations on the film morphology of polymer materials are demanding. In this talk, I will present recent results of joint theoretical and experimental studies of thiophene-rich polymer films⁵ and poly-(2,5-bis(3-alkylthiophene-2-yl)thieno[3,2-b]thiophene (pbTTT): phenyl-C₇₁-butyric acid methyl ester (PC71BM) bimolecular crystal.⁶ Possible polymer and polymer:fullerene blend structures will be suggested; on the basis of those structures, the various electronic properties of those film will be discussed. References 1.H. -Y. Chen et al. Nature photonics 3, 649 (2009) 2.Y.. Liang et al., Advanced Materials 22, E135 (2010) 3.Press Release Solarmer Energy Inc., July 27, 2010 4.Press Releases Konarka, November 29, 2010 5.R. Mondal et al., J. Mater. Chem. 20, 5823 (2010) 6.R. Gysel et al., MS in preparation

일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: **PHYS2-4**

발표분야: Computational Chemistry for Energy Materials

발표종류: 심포지엄, 발표일시: 금 10:40, 좌장: 김동욱

Origin of High Li-Storage in N-doped Graphitic Layers, and Electronic Structures of Porphyrin Nanoribbons

강홍석

전주대 나노신소재공학과

In this talk, I will describe my recent quantum mechanical calculations on the Li-storage in aromatic systems ranging from benzene, carbon nanotubes, to graphene bilayer. Specifically, atomistic origin of the experimental high Li storage capacity in N-doped graphitic layers will be clarified. In pyridinelike N-doped graphitic layers, we find that the high storage capacity is originated from the formation of dangling bonds around divacancy sites due to the rearrangement of carbon atoms, which is facilitated by a certain amount of prestored Li. In graphitic nitrogen-doped layers, monovacancies are also easily formed around the N-dopes sites upon Li-storage, which enhances the Li storage. In addition, I will also describe the origin of high efficiency in dye-sensitized solar cells based on a certain kind of dyes in terms of the electronic structure of those dyes. Furthermore, I will briefly describe the electronic structures of porphyrin-based polymer nanoribbons such as one-dimensional porphyrin tapes with various divalent metal ions as well as those of double-stranded porphyrin ladder polymers which can be potentially useful in light harvesting systems. Particularly, I will describe the discovery of "Giant Stark effect" in the ladder tape in detail, which is as strong as that recently found in boron nitride nanotube and nanoribbon.

일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: **PHYS2-5**

발표분야: Computational Chemistry for Energy Materials

발표종류: 심포지엄, 발표일시: 금 11:05, 좌장: 김동욱

Pillared Covalent Organic Frameworks with Balanced Volumetric and Gravimetric Hydrogen Uptake

최승훈

(주)인실리코텍

We propose the surface area and the free volume of the storage materials should be balanced to increase the gravimetric and volumetric hydrogen uptake capacities by modeling pillared covalent organic frameworks (PCOFs) with pyridine molecules inserted between the layers of COF-1. Density functional theory and grand canonical Monte Carlo calculations show that these PCOFs have significantly improved gravimetric and volumetric hydrogen storage capacities of 9.7 ~ 11.1 wt% and 58.7 ~ 62.5 g/L, respectively.

일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: **PHYS2-6**

발표분야: Computational Chemistry for Energy Materials

발표종류: 심포지엄, 발표일시: 금 11:30, 좌장: 김동욱

Multiscale features of Energy Materials: Computational Studies on DSSC and Li-ion Batteries

김형준, *전지원, **최정모, ***William A. Goddard III

KAIST EEWS 대학원 *KAIST EEWS **KAIST 화학과 ***California Institute of Technology

Many current scientists quest for the green and renewable energy materials to resolve the sustainability problem of Human beings. For chemists, especially for theoretical chemists, energy materials are also one of the most intriguing systems since many different types of chemistry (such as surface chemistry, electrochemistry, polymer chemistry, etc.) are simultaneously undergoing in these systems. In this talk, we demonstrate such a multiscale feature of energy materials and discuss our recent computational studies on the dye sensitized solar cells (DSSCs) and Li-ion batteries. DSSCs using imidazolium based ionic liquid (IL) as an electrolyte are known to have a better device stability than the systems using acetonitrile-based electrolyte, but the usage of IL degrades the power efficiency. Using molecular dynamics (MD) simulations with first principle based force-field parameters, we investigate the equilibrium liquid structure of electrolyte with transport properties to clarify the role of water molecules. This further leads a discussion about the optimal amount of water contents, which may enhance the power efficiency. For Li-ion battery systems, we first elucidate the crystal structure of C6O6-based organic cathode of which crystal structure has been discovered without clarifying the structure. Using a multiscale simulation approach based on the combination of density functional theory (DFT) and grand canonical Monte Carlo (GCMC), we determine the energetically favorable structure having same XRD peaks to the experimental results. Then, we show the temperature effect using ab-initio MD results. In the last part of the talk, we discuss the universal empirical correction method (low-gradient method) of van der Waal's interaction of DFT methods to investigate the lithiation mechanism of the graphite anode materials.

일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: ANAL1-7

발표분야: Novel Applications of Chromatography and Spectroscopy

발표종류: 분과기념강연, 발표일시: 목 16:40, 좌장: 한중훈

Effective analysis of proteins and carbohydrates using mass spectrometry

김정권

충남대 화학과

Mass spectrometer (MS) is frequently used in the analysis of proteins and carbohydrates. One of the bottlenecks in the analysis of proteins is the time required to digest protein samples to produce peptide mixtures. Generally, using in-solution digestion of a protein requires over 12 h. Various methods have been developed to reduce the digestion time, such as microwave, pressure, or ultrasound. Recently, we investigated pressure-assisted tryptic digestion using a 3mL-syringe, vortex-assisted tryptic digestion, and temperature effect on ultrasound-assisted tryptic digestion, where increased digestion efficiency was observed with the applied pressure, an increased vibrational speed and an ultrasound with higher temperature. During the presentation, various factors that are related to increasing tryptic digestion will be overviewed. The study on carbohydrates is important since carbohydrates play important roles in biological systems. Matrix-assisted laser desorption/ionization-mass spectrometry (MALDI-MS) is frequently used in the analysis of carbohydrates. However, MALDI-MS is known to be not a quantitative technique. In this presentation, quantitative analysis of chondroitin sulfate (CS) using MALDI-MS will be presented where relative quantitation of CS was performed by adding maltotriose (monoisotopic molar mass = 504.2) as an internal standard to the chondroitin ABC lyase-digested product of CS (N-acetylgalactosamine disaccharide units (monoisotopic molar mass = 503.0)). The relative ratio between the digested product of CS and maltotriose provided successful quantitative information.

일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: **ANAL1-1**

발표분야: Novel Applications of Chromatography and Spectroscopy

발표종류: 심포지엄, 발표일시: 목 14:00, 좌장: 임흥빈

Flow FFF & Nanoflow LC-ESI-MS-MS for Biological Macromolecules

문명희

연세대 화학과

FIFFF is an elution technique that can be utilized for pre-fractionating biomolecules such as proteins, cells, lipoproteins, and subcellular species by sizes. Introduced are the recent studies on the use of FIFFF as an alternative pre-analytical method for fractionating proteome followed by shotgun analysis of collected species after digestion or extraction using nanoflow liquid chromatography – electrospray ionization-tandem mass spectrometry (nLC-ESI-MS-MS). For the size fractionation of membrane proteins, glycosylated or phosphorylated proteins, FIFFF techniques such as hollow fiber FIFFF (HF5), frit inlet asymmetrical FIFFF (FI-AF4), and the isoelectric focusing-asymmetrical FIFFF (IEF-AF4) which is an on-line non-gel based two-dimensional (pI & hydrodynamic diameter) protein separation devices are utilized. This presentation also shows a potential utility of multiplexed HF5 and nLC-ESI-MS-MS for the lipidomics especially for the systematic profiling of various phospholipids (PLs) in lipoproteins from human blood plasma. Semi-preparative HF5 is utilized for the size fractionation of high density lipoproteins (HDL) and low density lipoproteins (LDL) from human plasma from coronary artery disease, and followed by the shotgun lipidomic analysis of different lipoproteins for the biomarker development.

일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: ANAL1-2

발표분야: Novel Applications of Chromatography and Spectroscopy

발표종류: 심포지엄, 발표일시: 목 14:25, 좌장: 임홍빈

Single Enzyme Molecule Study based on Single-Molecule Detection Techniques

강성호

경희대 응용화학과

Single-molecule detection can be used to directly observe individual steps or intermediates of biochemical reactions because stochastic events of individual molecules are masked in conventional measurements through ensemble averaging. Various scientific phenomena related to enzymology, including restriction enzymes, have also been explained at the single-molecule level. Thus far, however, single-molecule detection has been implemented successfully by using fluorescence detection and in rare cases electrochemical cycling. At first part, it was shown that chemiluminescence or bioluminescence detection could approach the single-molecule limit in sensitivity. In the second part, enzyme digestion of single-DNA molecules was directly observed in real time by dual-color total internal reflection fluorescence microscopy. Unlike previous studies, the length-based digestion rate of λ -exonuclease showed 3 distinct values. That is, different enzyme molecules exhibit different digestion dynamics.

일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: ANAL1-3

발표분야: Novel Applications of Chromatography and Spectroscopy

발표종류: 심포지엄, 발표일시: 목 14:50, 좌장: 임흥빈

Shotgun Lipidomics by Using Microfluidic Chip-based Mass Spectrometry

김영환

한국기초과학지원연구원 질량분석연구부

Lipids are essential cellular constituents that are multiple distinct yet critical roles as membrane bilayer, reservoirs for energy storage and the source of second messengers, in cellular function. The unique chemical structure of the majority of lipid molecular specie consists of linear combination of a small number of building blocks that include backbones, head groups, and aliphatic chains. Recently, shotgun lipidomics, to direct qualitative and quantitative analysis of complex mixtures of lipid by mass spectrometry have defined large-scale study, is a newly and rapidly expanding research field in system biology. In this study, phospholipids in mouse brain extracted with methyl-*tert*-butyl ether were analyzed by using microfluidic chip-based mass spectrometry. They were identified at the molecular species level by a combination of high resolution MS profiling and 'iLipid' program which was developed to search peak matching with lipid database. Their classification and fatty acyl compositions were also confirmed by using the precursor-ion scans of fragment ions specific to their polar head groups and neutral-loss scans of fatty acid carboxylate ions, RCOO^- , respectively.

일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: ANAL1-4

발표분야: Novel Applications of Chromatography and Spectroscopy

발표종류: 심포지엄, 발표일시: 목 15:25, 좌장: 박정학

Resolution of chiral and non-chiral compounds on various aminoalcohol derived π -acidic chiral stationary phases

류재정

경북대 화학교육과

Various aminoalcohol derived π -acidic chiral stationary phases (CSPs) were applied in resolving racemic N-acyl-1-naphthylaminoethanes and N-acetyl-1-naphthylaminoalkanes by chiral HPLC.[1] In this study, enantioseparation of racemic N-acyl-1-naphthylaminoisobutanes and N-acyl-1-(6,7-dimethyl)naphthylaminoethanes and polynuclear aromatic hydrocarbons (PAHs) on the same CSPs was performed and the chromatographic resolution results were compared. Based on the comparison of the resolution results on each CSP, the separation mechanism of N-acyl-1-naphthylaminoisobutanes and N-acyl-1-(6,7-dimethyl)naphthylaminoethanes and PAHs on these CSPs are proposed.[1] J.J. Ryoo, et al., J. Chromatogr. A, 987 (2003) 429.

일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: ANAL1-5

발표분야: Novel Applications of Chromatography and Spectroscopy

발표종류: 심포지엄, 발표일시: 목 15:50, 좌장: 박정학

Structural elucidation of complex organic mixture by mass spectrometry

김성환

경북대 화학과

Elucidation of molecular structure remains a great challenge for the study of complex organic mixture. In this study, mass spectrometric techniques have been used to get information on molecular structures of humic substance and petroleum compounds. Mass spectrometry may not be a method of choice to get molecular structure of compounds. NMR and X-ray crystallography have been more widely used for that purpose. However, mass spectrometry is the only technique that can resolve the complexity of organic mixture such as humic and petroleum compounds. Two mass spectrometric techniques have been employed for structural information. The first one is the ion mobility mass spectrometry (IM-MS). IM-MS separates gas-phase ions based on their relative mobility through a collision cell filled with an inert gas. Theoretical calculations indicated that mass mobility plot obtained by non-linear electric field IM-MS can be used for evaluating differences and similarity of structures in ion mobility spectra. From the mass mobility plot obtained by IM-MS analysis of crude oil, a trend where drift time changes with a given mass difference could be used to find structural similarity and difference in petroleum compounds. The concept was demonstrated using ion mobility mass spectra from a homologous series of compounds, differing only by the number of alkyl units, found in crude oil. The second technique used in this study is double bond equivalence (DBE) and carbon number distribution observed by high resolution mass spectrometry. Strong linear relationship between average DBE and carbon number vs number of oxygen in oxygenated compounds in humic substance has been observed. In this study, it is shown that the slope and intercepts of the linear relationship can be used to compare humic substance samples.

일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: ANAL1-6

발표분야: Novel Applications of Chromatography and Spectroscopy

발표종류: 심포지엄, 발표일시: 목 16:15, 좌장: 박정학

Quantitative Analysis of Lanthanides in High Temperature Molten salt by Using Laser-induced Fluorescence Spectroscopy

배상은, *박용준, *정의창, *송규석

한국원자력연구소 원자력화학연구부 *한국원자력연구원 원자력화학연구부

본 연구에서는 사용후핵연료 재활용을 위한 파이로 공정의 란타나이드 이온 정량 분석법 개발을 위하여 고온 용융염 내 녹아있는 란타나이드 이온의 시간분해 레이저 유도형광 (TRLFS) 과 흡수분광을 측정하였다. 고온 용융염에 녹아있는 Eu^{2+} , Sm^{2+} , Yb^{2+} 와 같은 란타나이드 이온들은 260 nm 영역에서 4f-5d 전이에 기인한 흡수띠뿐만 아니라 다양한 파장에서 각 원소의 특성 형광 신호를 나타냈다. Tb^{3+} 는 실온에서 873 K 사이의 모든 온도범위에서, $^5\text{D}_3$ 와 $^5\text{D}_4$ 준위로 여기된 전자의 $^7\text{F}_J$ ($J = 1, 2, 3, 4, 5, 6$) 준위로의 전이에 기인한 강한 형광 신호를 나타냈다. Nd^{3+} 는 가시광선 영역에서 4f-5f 전이에 기인한 여러 개의 흡수띠를 나타냈으나 Eu^{2+} 와 같은 원소에서 나타나는 4f-5d 전이의 흡수띠에 비해 매우 약한 세기를 보였다. Tb^{3+} 에서 관측된 형광의 경우 cross-relaxation 효과로 인해 $^5\text{D}_3$ 와 $^5\text{D}_4$ 준위에서 전이된 형광 신호가 변화하였으며 Nd^{3+} 의 경우 concentration quenching 효과에 의해 농도가 증가함에 따라 600 nm 영역의 형광신호는 감소하고 810 nm 영역의 형광신호는 증가하였다. 고온 용융염 내 란타나이드 이온들의 형광띠 결과를 이용하여 농도에 따른 형광 세기의 선형 검정곡선을 구하였다. 그 결과에 따르면 TRLFS 가 파이로 공정의 란타나이드 이온 실시간 정량 분석 기술로 유용한 것으로 판단되었다.

일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: ANAL2-1

발표분야: Emerging Nanobiotechnologies in Analytical Chemistry

발표종류: 심포지엄, 발표일시: 금 09:10, 좌장: 이광필

Surface enhanced Raman scattering based on micro gold shells for advanced chemical analysis

정택동

서울대 화학부

As one of the most promising candidates to possibly monitor chemical environment in situ during electrochemical reactions or biological events, Raman scattering has a critical drawback, sensitivity. That is why a great deal of efforts have been made to find the way to use Raman spectroscopy for this purpose by enhancing the light scattering intensity. In this respect, surface enhanced Raman scattering(SERS) has been attracting keen attention, focussing on better substrates that is the key factor to accomplish its practical utility as an analytical tool. We have been pursuing new SERS substrates based on thin gold shells covering micro polymeric beads. As a fruit, sophisticatedly engineered micro gold shells are available for SERS-based analysis of molecular sub monolayers on conducting or non-conducting substrates. Moreover, a single micro gold shell can be used to be an ultramicroelectrode(UME) for scanning electrochemical microscope(SECM). The hybrid probe as made is expected to provide a new way to monitor the chemical release on local site of an biological sample, to screen the activity of electrocatalysts, and to pattern the metal or biological molecules onto the specific sites by Raman scattering as well as electrochemistry simultaneously. This talk will show how creatively microfluidic technology can be combined with SERS for modern analytical chemistry.

일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: ANAL2-2

발표분야: Emerging Nanobiotechnologies in Analytical Chemistry

발표종류: 심포지엄, 발표일시: 금 09:35, 좌장: 이광필

Endogenous peptidomic analysis and top-down proteomic analysis by use of nanoLC-FTMS

이지은

KIST 도핑콘트롤센터

Fourier transform mass spectrometry (FTMS) provides unique benefits of complete identification and characterization of peptides and proteins, including posttranslational modifications (PTMs) because of its ultrahigh mass accuracy and resolution. Here, we performed endogenous peptidomic analysis and top-down proteomic analysis by use of nanocapillary reversed-phase liquid chromatography (RPLC) on a 12 Tesla FTMS. First, the suprachiasmatic nucleus (SCN) located at the base of the hypothalamus, contains the master circadian clock, synchronizing the body's circadian rhythms. While peptides present in the SCN are known as critical synchronizers and mediators of normal SCN functions, there have not been yet any comprehensive peptidomic studies of the SCN by mass spectrometry (MS). We performed the first peptidomic study of the rat SCN tissue punches by use of FTMS/MS. The high-resolution FTMS coupled with tailored software produced a hyper-confident list of 102 endogenous peptides, including PTMs. Second, while top-down proteomics in which hundreds of intact proteins are fragmented directly in a mass spectrometer allows extensive characterization of the proteins, effective separation of intact proteins is absolutely critical to reduce sample complexity and obtain higher proteome coverage in top-down proteomics. Here, we employed an intact protein separation scheme based on molecular weight known as gel-eluted liquid fraction entrapment electrophoresis (GELFrEE) before top-down mass spectrometry of complex mixtures. GELFrEE and online nanocapillary RPLC coupled to tandem mass spectrometry allowed for a high throughput format of top-down proteomic analysis in a fashion similar to that of bottom-up proteomics.

일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: ANAL2-3

발표분야: Emerging Nanobiotechnologies in Analytical Chemistry

발표종류: 심포지엄, 발표일시: 금 10:00, 좌장: 이광필

Small-Molecule-Tagged Gold Particles for Biosensing and Tissue Imaging by MALDI-TOF MS

여운석

건국대 생명공학과

It has been of great interest developing tools and methods to control and detect molecular level interactions between materials and biological systems. Recently, various types of nanomaterials with bio-functionalized, chemically tailored, and structurally well defined surfaces have been widely used for standardized diagnostic tools, biosensors, and new analytical systems. In this talk, I will introduce small-molecule-tagged gold particles and their application for biosensing and tissue imaging by combining self-assembled monolayers (SAMs) on gold and LDI-TOF MS. In the first example, biological signals are transduced to amplified mass signals allowing ultrasensitive detections of target of interest in solution such as antigens, microRNA, insecticide, and antibiotics. The strategy does not require the use of labels and therefore avoid complicated, additional steps for labeling. The second application describes a matrix-free format tissue imaging utilizing hollow gold nanoparticles which are modified with capture proteins such as antibodies. The antibody modified HGNs are specifically bound to the biomarker expressed on cancerous tissue. HGN carries a number of small molecules which are subsequently analyzed by LDI-TOF MS. In this way, the mass spectra give the spatial distribution of the biomarker on the tissue. Our strategy to image biological tissues without organic matrix is especially attractive for cell or biological tissue imaging because we observe small molecules instead of huge biomolecules and hence it allows improved resolution and quantitative information.

일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: ANAL2-4

발표분야: Emerging Nanobiotechnologies in Analytical Chemistry

발표종류: 심포지엄, 발표일시: 금 10:35, 좌장: 정희일

Force-Based AFM for Protein Analysis at Single Molecule Level

박준원

포항공과대 화학과

Second-generation and third-generation dendrons have been applied to AFM probes and substrates to control spacing between the immobilized biomolecules on them. For DNA-DNA interaction, both binding and unbinding events were recorded, and enhanced sharpness of the force histograms was an additional advantage from the controlled surface. The same approach has been employed to reveal thermodynamic behaviour of a folded nano- π -stack, a model protein, and to study the specific interactions between the signal transducing proteins mammalian phospholipase D1, phospholipase C- γ 1, and Munc-18-1. Recently, we have shown that individual captured PSA on the protein microarray surface can be imaged and counted one by one. This new progress enabled us to measure the concentration of the protein biomarker in the range that is beyond of ELISA, and obtain the affinity constant of a signal transducing protein at single molecule level.

일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: ANAL2-5

발표분야: Emerging Nanobiotechnologies in Analytical Chemistry

발표종류: 심포지엄, 발표일시: 금 11:00, 좌장: 정희일

Recent Advances in Surface Plasmon Resonance Biosensing

정봉현

한국생명공학연구원 바이오나노연구센터

Surface plasmon resonance (SPR) is an optical technique used to detect the specific binding of unlabeled bio-molecules onto molecules attached to chemically modified gold thin films by measuring changes in the index of refraction upon adsorption. Furthermore, it has also been used as a valuable tool to investigate molecular interactions in real time without the use of labels. In principle, SPR is highly sensitive to changes in the refractive index close to metal surfaces. Therefore, one can detect the binding of biochemical molecules with high sensitivity on the surface in real time. Gold surface-based SPR has been used to detect diverse biological substances (e.g., proteins, DNA, small organic molecules, toxins and viruses) for a wide range of applications (e.g., drug screening, disease immunoassays, process control, and environmental monitoring). To date, numerous attempts have been made to enhance the performance and sensitivity of SPR-based detection technology, resulting in the development of SPR sensor systems for satisfying the requirements of various industrial and research areas. In this presentation, the primary issues of SPR biosensing will be addressed, and also our recent studies to improve the performance of SPR biosensing will be introduced. In addition, I will present a novel miniaturized SPR sensing scheme with the palm-sized SPR biochemical sensor which is devised in our lab.

일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: ANAL2-6

발표분야: Emerging Nanobiotechnologies in Analytical Chemistry

발표종류: 심포지엄, 발표일시: 금 11:25, 좌장: 정희일

Fully Integrated Lab-on-a-disc for Biomedical Applications

조윤경

울산과학기술대 나노생명화학공학과

We report fully automated "lab-on-a-disc" systems for various biomedical applications. Raw samples such as whole blood, saliva, urine can be directly applied to the disc and the necessary reaction steps are all integrated on a disc. Using the innovative laser irradiated ferrowax microvalves together with the centrifugal microfluidics, the total process of separation, metering, mixing, incubation, washing, and detection is fully automated using a small portable device. The analyzer is also equipped with an optical detection module to measure absorbances at 10 different wavelengths to accommodate the various kinds of reaction protocols. In this paper, we report various kinds of biomedical applications integrated on a disc such as PCR-ready DNA extraction from virus or bacteria starting from whole blood, multiplex immunoassay starting from whole blood or saliva, simultaneous analysis of multiple blood chemistry and immunoassay from whole blood. Compared to the conventional analysis done in clinical laboratories, it is advantageous for point-of-care applications because it requires a smaller amount of blood (~100 μ L vs 1 mL), takes less time (~ 20 min vs several days), does not require specially trained operators or expensive instruments.

일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: ANAL2-7

발표분야: Emerging Nanobiotechnologies in Analytical Chemistry

발표종류: 심포지엄, 발표일시: 금 11:50, 좌장: 정희일

Highly Sensitive Biomedical Diagnosis Using Nanoprobe-based Optofluidic Sensor

주재벌

한양대 생명나노공학과

Metal nanoparticle is emerging as one of the most effective optical detection tools in nanobiotechnology. Depending on their chemical composition, their optical properties have garnered much attention in biological studies approaching molecular dimensions. In this presentation, a SERS-based optofluidic system for fast and sensitive immunoassay, will be presented. The microfluidic channel used here is composed of three components: the gradient channel that serially dilutes the target marker, the injection and mixing part of magnetic beads and HGNS, and the trapping part of the sandwich immunocomplexes using multiple solenoids. The potential immunoanalytical capability of this system has been evaluated for various cancer and cardiac markers. This novel SERS-based optofluidic immunoassay system is expected to be a powerful clinical tool for the fast and sensitive medical diagnosis of a disease.

일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: BIO1-1

발표분야: Recent Development of Nanobio Technology

발표종류: 심포지엄, 발표일시: 목 14:00, 좌장: 윤문영

Development and application of smart biomaterials for non-viral gene therapy

김원중

포항공과대 화학과

Gene therapy has attracted enormous attention over the past few decades due to its immense potential as a therapeutic tool for combating various genetic disorders. Among two kinds of vectors that are employed till date, viral vectors exhibit higher transfection efficiencies, but their use is impaired greatly due to the associated toxicity, immunogenicity, and non-viable scale up procedures. As a result, tremendous impetus has been directed toward the development of various nonviral synthetic delivery systems which could be safer and more efficient. A number of cationic polymers including polyethylenimine (PEI), chitosan, and poly(L-lysine) have also been reported to exhibit efficient gene transfection. However, the induced cytotoxicity and non-biodegradability of these cationic polymeric vectors along with inefficient release of gene from the polymeric complexes inside the cell, lack of target specificity impede the prevalent practical realization of gene therapy. Therefore, in our quest to develop a highly coveted vector which could provide all these attributes, we have devised several highly efficient vector systems. Our approaches are focused mainly on the development of smart nanoparticles which could exploit the intracellular and extracellular features of the target cells by imparting several structural or functional traits into the nanoconstructs in order to overcome various impediments.

일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: **BIO1-2**

발표분야: Recent Development of Nanobio Technology

발표종류: 심포지엄, 발표일시: 목 14:30, 좌장: 윤문영

Novel in vitro protein producing gel matrix for functional and therapeutic antibodies

엄승호

광주과학기술원 신소재공학과

Owing to the biocompatibility and specific selectivity, nucleic acids such as DNA and RNA have been recognized as a generic building block and thus they're self-assembled into nanoarchitectures like cube, tetrahedron, triangle, origami or three-dimensional constructs like DNA based hydrogel. Combined with genetic codes, the DNA hydrogel can produce functional proteins without any living cells. This protein-producing gel (which is also called as 'the P-gel system' or 'P-gel') consists of DNA building blocks and genes as parts of the gel scaffolding. The product efficiency was about 300 times higher than current, solution-based systems. It is proved that the mechanisms behind the high efficiency and yield may be due to improved gene stability and a faster enzyme turnover rate resulting from a closer proximity of genes. P-gels containing a total of 16 different genes have been tested and successfully produced all 16 proteins including hard-to-express-in-cell proteins. It demonstrates that novel P-gel system can serve as a protein producing and amplifying platform technology.

일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: **BIO1-3**

발표분야: Recent Development of Nanobio Technology

발표종류: 심포지엄, 발표일시: 목 15:00, 좌장: 윤문영

Highly Sensitive Biohybrid Nanoprobes for Surface Enhanced Raman Scattering Based Biosensing and Bioimaging

임동우

한양대 생명나노공학과

Surface Enhanced Raman Scattering (SERS) has been of great interest to develop highly sensitive biosensors and bioimaging instruments based on optical detection. In this study, various SERS biohybrid nanoprobes with clustered silver nanoparticles were synthesized to detect specific biological moieties with ultra-sensitivity. Raman dye induced aggregation of silver nanoparticles dramatically increased SERS signal many orders higher than individual silver nanoparticles due to electromagnetic enhancement at highly localized plasmonic centers on the rough metal substrate. Those clustered silver nanoparticles were encapsulated into the polymeric nanoparticles or nanofibers via electrohydrodynamic jetting and then chemically-stabilized. The SERS intensity was largely controlled by density of the clustered silver nanoparticles within the polymeric nanoparticles. These SERS nanoprobes were biocompatible and chemically stable in the wide range of pH and ionic strength due to chemical crosslinking. Furthermore, a variety of biological moieties were introduced on the surface of the SERS nanoprobes to detect specific cell markers for multiplexing system. Controllable SERS intensity, high sensitivity, chemical stability, biocompatibility, signal reproducibility as well as large-scale synthesis at a low cost make the biohybrid SERS nanoprobes useful for biosensing and bioimaging applications.

일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: **BIO1-4**

발표분야: Recent Development of Nanobio Technology

발표종류: 심포지엄, 발표일시: 목 15:50, 좌장: 임태연

Immune cells-specific delivery of Mannan-coated magnetic Nanoparticles for Diagnosis of micro-metastasis

박인규

전남대 의생명과학과

Detection of lymph node (LN) metastasis by magnetic resonance imaging (MRI) has obtained clinical significance for treating cancer patients. LN metastasis often happens through regional lymphatic system, leading to distal tumor formation including lungs, liver and bones. Successful imaging of small and microscopic LN metastasis provides the helpful information in deciding the therapeutic option of cancer. Mannan is a water-soluble polysaccharide having high content of D-mannose residues which can be recognized by mannose receptors on activated macrophages and dendritic cells. Mannan-coated superparamagnetic iron oxide nanoparticles (Mannan-SPION) were developed to be specifically delivered to macrophages in lymph node by receptor-mediated endocytosis. Mannan-SPION was proven to be suitable for MR imaging due to small size, excellent stability in ferrofluid, and low cytotoxicity. In addition, mannan-SPION exhibited enhanced targeted delivery efficiency to macrophages in lymph nodes in vivo compared with PVA-SPION. Especially, LN enhancement of Mannan-SPION on MRI was dramatically increased at the later stage after intravenous injection compared with PVA-SPION control, indicative of the potential to successfully detect micrometastasis in LN.

일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: **BIO1-5**

발표분야: Recent Development of Nanobio Technology

발표종류: 심포지엄, 발표일시: 목 16:20, 좌장: 임태연

Combinational RNAi for enhanced anti-tumor efficacy

이상경

한양대 생명공학과

The RNAi technology has great potential for use in cancer therapy and a plethora of genes have been identified and evaluated as effective RNAi targets. However, tumor regression is highly dependent on the type and the stage of cancer, the gene target chosen for silencing and the method of RNAi-drug delivery. We have investigated whether the efficacy of siRNAs in cancer therapy could be improved by the simultaneous blockade of several gene products and pathways implicated in cancer biogenesis. We chose to target the gene products of bcl-2, c-Myc and VEGF that are frequently overexpressed in multiple tumors, including melanomas. Further we use a novel polymer – a arginine-grafted bioreducible polydisulfide amine (ABP) with increased siRNA encapsulating properties and reduced toxicity for siRNA delivery. Combinatorial treatment with all three siRNAs not only allowed extended control of B16.F10 melanoma cell proliferation in culture but also in vivo in a mouse model of solid tumor engraftment. Intratumoral injection with a siRNA cocktail targeting the three genes almost completely regressed a larger tumor volume in contrast to single or dual siRNA treatments. Further, systemic intravenous administration of the ABP/siRNA cocktail enabled enhanced permeability and retention (EPR) with a significant anticancer activity. Our results suggest that multiplexing siRNAs can results in a synergistic inhibitory effect on cancer progression and combination therapy incorporating multiple RNAi targets with current modalities would vastly improve the prognosis of cancer.

일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: **BIO1-6**

발표분야: Recent Development of Nanobio Technology

발표종류: 심포지엄, 발표일시: 목 16:50, 좌장: 임태연

Novel Flow Cytometric Techniques for Analysis of Protein Phosphorylation and Signaling Networks

김유찬

BD Korea

Intracellular evaluation of signaling systems has been limited by an inability to correlate active protein states to functional subsets of cells within the native context of the cell. Multi-dimensional flow-cytometric analysis of these active protein states via phospho-epitope recognition, in combination with surface marker staining and other detectable parameters (ie, intracellular cytokines, apoptotic changes), can provide functional assessment at a single cell level that may have utility in clinical diagnostics and/or disease progression monitoring. Furthermore, the ability to profile both activating and inhibiting conditions of multiple protein states simultaneously within the cell in a rapid and parallel manner may be extended to screening of compounds or other pharmaceutical applications.

일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: **BIO2-1**

발표분야: Researches and Applications of Protein Chemistry

발표종류: 심포지엄, 발표일시: 금 09:00, 좌장: 임용범

Crystallographic and mutational analysis of the CD40-CD40L complex.

이지오

KAIST 화학과

CD40 is a tumor necrosis factor receptor (TNFR) family protein that plays an important role in B cell development. CD154/CD40L is the physiological ligand of CD40. We have determined the crystal structure of the CD40-CD154 complex at 3.5 Å resolution. The binding site of CD40 is located in a crevice formed between two CD154 subunits. Charge complementarity plays a critical role in the CD40-CD154 interaction. Some of the missense mutations found in hereditary hyper-IgM syndrome can be mapped to the CD40-CD154 interface. The CD40 interaction area of one of the CD154 subunits is twice as large as that of the other subunit forming the binding crevice. This is because cysteine-rich domain 3 (CRD3) of CD40 has a disulfide bridge in an unusual position that alters the direction of the ladder-like structure of CD40. The Ser132 loop of CD154 is not involved in CD40 binding but its substitution significantly reduces p38- and ERK-dependent signaling by CD40, while JNK-dependent signaling is not affected. These findings suggest that ligand-induced di- or tri-merization is necessary but not sufficient for complete activation of CD40.

일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: **BIO2-2**

발표분야: Researches and Applications of Protein Chemistry

발표종류: 심포지엄, 발표일시: 금 09:25, 좌장: 임용범

Protein Structure Prediction by Global Optimization and its Applications

이주영

고등과학원/계산과학부

One of the fundamental goals of modern sciences is to understand the nature of life, and deciphering the protein structure and its working mechanism lies at the very heart of this agenda. Due to the tremendous success of many genome projects, the number of available protein sequences reached over 5.3 million as of 2007, but less than 1% of these protein structures are known. Reliable and accurate protein structure prediction using only the sequence information is greatly in demand, but it remains as an unsolved problem even after many years of efforts. We intend to establish a successful protein modeling method that is solely based on direct application of principles excluding human interference in modeling steps. This should be contrasted to the common conception in the field that human expertise accumulated by many years of protein modeling is the most important asset for accurate protein structure prediction. In this talk we will discuss recent progresses of our efforts in protein structure prediction. It appears that our newly proposed method, which is based on the direct and rigorous optimization of relevant score functions, can provide significantly improvement for 3D modeling of proteins in the category of High-Accuracy Template-Based Modeling. Applications of highly accurate proteins 3D models to various biological systems will be discussed. Acknowledgments: Computation was carried out using KIAS Supercomputers and this work was supported by Korea Science and Engineering Foundation (KOSEF) and Korea government (MEST) by the grant number: 2009-0063610. References [1] Keehyoung Joo, Jinwoo Lee, Sunjoong Lee, Joo-Hyun Seo, Sung Jong Lee, and Jooyoung Lee, Proteins 69, 83-89 Suppl. 8 (2007). [2] Keehyoung Joo, Jinwoo Lee, Ilsoo Kim, Sung Jong Lee and Jooyoung Lee, Biophys. J. 95, 4813-4819 (2008). [3] Keehyoung Joo, Jinwoo Lee, Joo-Hyun Seo, Kyoungrim Lee, Byung-Gee Kim, Jooyoung Lee, Proteins 75, 1010-1023 (2009). [4] Elmar Krieger, Keehyoung Joo, Jinwoo Lee, Jooyoung Lee, Srivatsan Raman, James Thompson, Mike Tyka, David Baker, and Kevin Karplus, Proteins 77, 114-

122 Suppl. 9 (2009). [5] Mina Oh, Keehyoung Joo, Jooyoung Lee, Proteins 77, 152-156 Suppl. 9 (2009).[6] Jae-Sung Woo, Jae-Hong Lim, Ho-Chul Shin, Min-Kang Suh, Bonsu Ku, Kwang-Hoon Lee, Keehyoung Joo, Howard Robinson, Jooyoung Lee , Sam-Yong Park, Nam-Chul Ha and Byung-Ha Oh, Cell 136, 85-96 (2009).



일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: **BIO2-3**

발표분야: Researches and Applications of Protein Chemistry

발표종류: 심포지엄, 발표일시: 금 09:50, 좌장: 임용범

Autodisplay Technology for Biosensor Applications

변재철

연세대 신소재공학부

For the realization of immunoaffinity (IA) biosensors, antibodies have been usually immobilized on the metal surface of transducers as a molecular recognition layer. As the antigen-binding sites of antibodies are located at Fab region, the sensitivity of the IA biosensors is influenced on the orientation of antibodies. In this work, Z domain of protein A with IgG-binding activity was expressed on the outer membrane of E.coli as a fusion protein of AIDA-1 by using Autodisplay method. The outer membrane of E.coli with Z-domain was isolated to be colloid particle with a diameter of 100 nm. The prepared E.coli outer membrane was coated on the gold surface and the IgG-binding activity was tested by the binding assay with fluorescence labeled IgG. In comparison to the intact outer membrane, the outer membrane with Z-domain showed significant amount of IgG binding activity. The outer membrane of E.coli with Z-domain was treated to the gold surface of SPR biosensor. After anti-hIgG antibodies were immobilized to the Z-domain, hIgG antibodies were measured as a target analyte. This work presents that the outer membrane of E.coli with Z-domain could increased the sensitivity of SPR biosensor through the orientation control of antibodies at the molecular recognition layer.

일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: **BIO2-4**

발표분야: Researches and Applications of Protein Chemistry

발표종류: 심포지엄, 발표일시: 금 10:15, 좌장: 임용범

Self-Assembly of Artificial Protein Fragments: Folding into Shape

이희승

KAIST 화학과

Biological functions commonly hinge on the ability of small molecules to self-assemble into complex functional systems through intermolecular interactions. Looking to mimic these natural systems and understand the mechanism that governs their assembly, we have recently developed a method for producing molecular architectures using artificial protein fragments, β -peptides, as building blocks. The self-assembly process resembles protein folding in biological systems.

일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: **BIO2-5**

발표분야: Researches and Applications of Protein Chemistry

발표종류: 심포지엄, 발표일시: 금 10:40, 좌장: 이희승

Structural Studies of SARAH Domains from Mst1 and RASSF Family Proteins

정재준

한국기초과학지원연구원 자기공명연구부

In eukaryotic cells, apoptosis and cell cycle arrest by the Ras RASSF MST pathway are controlled by the interaction of SARAH (for Salvador/Rassf/Hippo) domains in the C-terminal part of tumor suppressor proteins. The Mst1 SARAH domain interacts with its homologous domain of Rassf1 and Rassf5 (also known as Nore1) by forming a heterodimer that mediates the apoptosis process. Here we describe the homodimeric structure of the human Mst1 SARAH domain, and its heterotypic interaction with the Rassf5 SARAH domain. The Mst1 SARAH structure forms a homodimer containing two helices per monomer. An anti-parallel arrangement of the long alpha helices (h2/h2') provides an elongated binding interface between the two monomers, and the short 310 helices (h1/h1') are folded toward that of the other monomer. Chemical shift perturbation experiments identified an elongated, tight binding interface with the Rassf5 SARAH domain, and a 1:1 heterodimer formation. The linker region between the kinase and the SARAH domain is shown to be disordered in the free protein. This implies a novel mode of interaction with RASSF family proteins, and provides insight into the mechanism of apoptosis control by the SARAH domain. If time permits, MR microimaging and MR animal imaging studies will be presented. With an advancement of magnetic resonance technology, we could follow developmental events from as early as the first cleavage stage to the early tailbud stage sequentially. Temporal and spatial resolutions have been improved, and consequently subcellular dynamic events inside an embryo during development could be revealed.

일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: **BIO2-6**

발표분야: Researches and Applications of Protein Chemistry

발표종류: 심포지엄, 발표일시: 금 11:05, 좌장: 이희승

Development of Biomolecular Modeling Methods and Applications to Biochemistry Problems

석차욱

서울대 화학부

In this presentation, I will describe the molecular modeling tools developed in our lab and the application studies performed using these and other available tools. We have developed a template-based protein structure prediction method, protein loop modeling methods, and protein-ligand and protein-protein docking methods. The main emphasis during the development of these modeling tools has been in effective combination of physics-based potentials and knowledge-based potentials such that native-like states are found by efficient global optimization. Our application studies include modeling of transmembrane proteins, protein-DNA complexes, and redox-sensitive ZAS (zinc-binding anti-sigma factor) proteins. A recent modeling study on the molecular origin of the redox-sensitivity of ZAS proteins will be discussed in more detail.

일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: **BIO2-7**

발표분야: Researches and Applications of Protein Chemistry

발표종류: 심포지엄, 발표일시: 금 11:30, 좌장: 이희승

Self-Assembling Nano-Proteins from Peptides

임용범

연세대 신소재공학과

Proteins are perhaps one of the most diverse and complex structures in nature. Functional diversity of proteins is very broad. Proteins, similarly to synthetic polymers, are in fact polymeric molecules. Proteins, however, have many unique characteristics compared to synthetic polymers. One of the most salient features of proteins is that each proteins form unique three dimensional structures, which is determined by their amino acid sequences. When compared to synthetic polymers, another important characteristic feature of proteins is the monodispersity in molecular weight. Due to the monodisperse property, lot-to-lot variation can be minimized between different preparations. Moreover, with rapidly expanding repertoire of non-natural/synthetic amino acids in recent years, we can modify the function and structure of natural proteins for our own needs or design entirely new ones. Self-assembling peptide nanostructures can mimic or displace the diverse biological functions of natural proteins with enhanced properties or with functions unprecedented in nature. Self-assembling peptide nanostructures are constructed by using bottom-up process. Therefore, conventional knowledge of self-assembly processes and nanotechnology techniques can be applied when developing self-assembling peptide nanostructures. In addition, natural principles on protein folding/self-assembly can give valuable inspiration to the construction of artificial self-assembling peptide nanostructures. In this regard, self-assembling peptide nanostructures can be referred to as "artificial protein nanostructures/nanomaterials". In this talk, our recent works on the self-assembling peptide nanostructure development is presented.

일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: **ORGN1-1**

발표분야: International Symposium on Organic Chemistry (1) : Recent Developments on the Catalysis and Natural Product Synthesis

발표종류: 분과기념강연, 발표일시: 목 13:30, 좌장: 안광현

Navigation in Biologically Relevant Chemical Space

김상희

서울대 약학대학/약학과

Chemical space is infinite and limited only by the chemist's imagination. Within chemical space, biologically relevant chemical space is amazingly small compared to the possible chemical space. Although it is small, some estimates of this number are in excess of 10⁶⁰. This number is huge far more than we can comprehend. We chemist have a rich array of skills and techniques with which we can create or discover small organic compounds that can be used for biological systems. Despite such expert knowledge, the registered number of small organic compounds is only around 2x10⁷. This number is insufficient to examine the entire biological space. Indeed, it is practically impossible and irrelevant to build the complete biologically relevant chemical space. Thus, scientists have been guided by Nature in navigating biologically relevant chemical space to identify regions containing relevant bioactive compounds. The possibility that natural products and endogenous compounds will be biologically relevant is very high, since they are evolutionarily selected, biologically pre-explored, and validated by Nature. Understanding the link between natural/endogenous products and biological space prompted us to explore the biologically relevant chemical space through chemical modification to understand the fundamental processes of life and to develop new strategies for identifying potential drug candidates. In this presentation, I would like to share our current efforts on this field. This involves the synthesis of natural/endogenous products, design and evaluation of their mimetics, and preparation of natural product-like compounds library.

일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: **ORGN1-2**

발표분야: International Symposium on Organic Chemistry (1) : Recent Developments on the Catalysis and Natural Product Synthesis

발표종류: 심포지엄, 발표일시: 목 14:00, 좌장: 허정녕

Synthesis of Bifunctional Allylboron Reagents via Allene Hydroboration Reactions, and Applications to the Synthesis of Biologically Active Natural Products

William R. Roush

The Scripps Research Institute, U.S.A.

This lecture will focus on the development new generations of bifunctional allylboron reagents via the hydroboration of allenes. These new reagents have led to a substantial expansion of the scope of the double allylboration reaction first reported from our laboratory in 2002. Application of these new reagents to the total synthesis of biologically active natural products will also be presented.

일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: **ORGN1-3**

발표분야: International Symposium on Organic Chemistry (1) : Recent Developments on the Catalysis and Natural Product Synthesis

발표종류: 심포지엄, 발표일시: 목 14:40, 좌장: 허정녕

Development of Enyne Metathesis and Metallotropic Shift for the Synthesis of Compounds with Multiple Un saturations

Daesung Lee

University of Illinois at Chicago, U.S.A.

Enyne metathesis is a powerful subclass of olefin metathesis that possesses a significant potential in organic synthesis. In light of developing new concepts and strategies for the construction of molecular structures containing unsaturated functionalities, we have been exploring enyne metathesis in ring-closing and cross metathesis formats in conjunction with a closely related process known as metallotropic [1,3]-shift. In this presentation, the recent progress of enyne metathesis and metallotropic [1,3]-shift and their application to total synthesis of various natural products will be discussed along with the discovery of new types of stable ruthenium alkylidene complexes.

일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: ORGN1-4

발표분야: International Symposium on Organic Chemistry (1) : Recent Developments on the Catalysis and Natural Product Synthesis

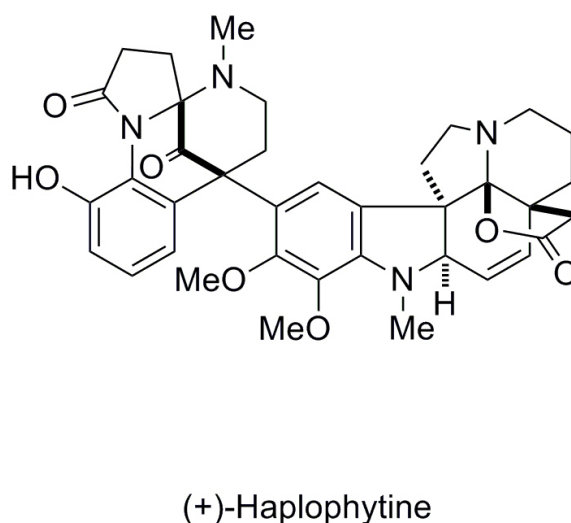
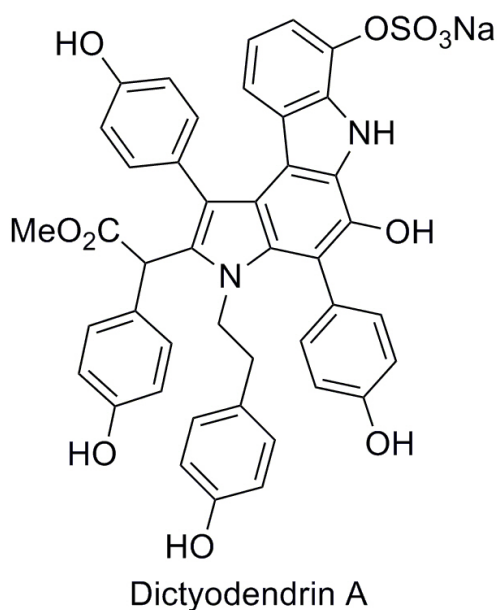
발표종류: 심포지엄, 발표일시: 목 15:15, 좌장: 허정녕

New Synthetic Strategy for Nitrogen Heterocycles and Its Application to Total Synthesis of Structurally Complex Alkaloids

Hidetoshi Tokuyama

Tohoku University, Japan

Total syntheses of two different types of architecturally complex indole alkaloids based on the development of novel synthetic strategies for nitrogen heterocycles will be discussed. For the synthesis of dictyodendrins, we have devised a novel one-pot benzyne-mediated indoline formation-cross coupling sequence, which provided the key intermediate for the efficient modular synthesis of dictyodendrins A to E.¹ The second topic will deal with the first total synthesis of a dimeric indole alkaloid, haplophytine, featuring an arylation reaction at the indole 4a position and an oxidative semi-pinacol type rearrangement of the 1,2-diaminoethene derivative to construct the spiro-aminal structure.²



일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: ORGN1-5

발표분야: International Symposium on Organic Chemistry (1) : Recent Developments on the Catalysis and Natural Product Synthesis

발표종류: 심포지엄, 발표일시: 목 16:10, 좌장: 이철범

Catalytic C-H Functionalization of Heterocycles for the C-C and C-N Bond Formation

장석복

KAIST 화학과

Silver-mediated intermolecular amination reactions of benzoxazoles were developed using formamides or parent amines as an amino group source. While the reaction with formamides requires rather harsh conditions, that with parent amines proceeds under milder conditions to afford 2-aminobenzoxazoles in high yields. Optically active amino groups could also be installed without racemization and significance of the present direct amination was demonstrated in one step synthesis of a biologically active coumarinyl benzoxazole derivative. It is proposed that formamides are first decarbonylated by the action of carboxylic acid additives to afford amines (or their salts) that subsequently react with protonated benzoxazoles leading to a putative 2-amino-benzoxazoline intermediate. Rearomatization of could be facilitated by silver species presumably through a single electron transfer to afford 2-aminated product at the end. Kinetic isotope competition studies revealed that the intermolecular kinetic isotope effects (KIE) being 0.9, thereby implying that a silver-mediated C-H activation pathway is less likely. A new catalytic system of the cobalt or manganese species in combination with peroxide and acid additive has been developed for the direct amination of azoles with amines. The reaction is highly attractive from the synthetic point of view in that the catalyst loadings are low, optimal conditions are highly mild, and substrate scope is broad.

일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: **ORGN1-6**

발표분야: International Symposium on Organic Chemistry (1) : Recent Developments on the Catalysis and Natural Product Synthesis

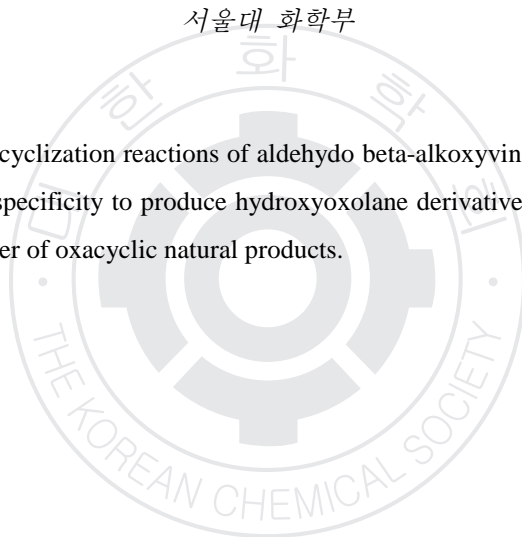
발표종류: 심포지엄, 발표일시: 목 16:45, 좌장: 이철범

Synthesis of Oxacyclic Natural Products: Recent Progress

이은

서울대 화학부

Samarium iodide-mediated cyclization reactions of aldehydo beta-alkoxyvinyl sulfoxides proceed in high stereoselectivity and stereospecificity to produce hydroxyoxolane derivatives. This reaction may be used in total syntheses of a number of oxacyclic natural products.



일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: ORGN2-1

발표분야: International Symposium on Organic Chemistry (2) : Recent Developments on Organic Functional Materials

발표종류: 심포지엄, 발표일시: 금 14:00, 좌장: 이희승

Smart Polymer Applications in Drug Delivery and Diagnostics

Allan S. Hoffman

University of Washington, U.S.A.

In the first part of my talk I will describe our work with smart polymer carriers for intracellular delivery of biomolecular drugs. Such drugs include peptides, proteins and nucleic acid drugs (eg, pDNA and siRNA). Many of these drugs act at intracellular sites; however, the effective intracellular delivery of these “fragile” drugs remains a significant challenge. Endocytosis of drug formulations usually results in localization within the endosome, where the predominant fate is fusion with lysosomes and enzymatic degradation of the biomolecular drug. Inspired by the principle behind the ability of many viruses to deliver their genomic cargo from the endosome to the cytosol, we have designed and synthesized a family of biomimetic, “smart” acid-responsive polymeric carriers that can enhance the escape of fragile biomolecular drugs from the endosome to the cytosol. In the second part of my talk I will describe our application of smart T- and pH-responsive polymers for point-of-care immunoassays. In this work, we have synthesized smart polymers using RAFT polymerization techniques, and conjugated them to: a) capture antibodies, b) porous membrane surfaces, c) magnetic and d) gold nanoparticles. We have also coated the smart polymer-antibody conjugates on magnetic and gold nanoparticles. These smart polymer systems are used to capture and concentrate the target, biomarker molecules and then release them as a concentrated pulse for downstream assay.

일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: ORGN2-2

발표분야: International Symposium on Organic Chemistry (2) : Recent Developments on Organic Functional Materials

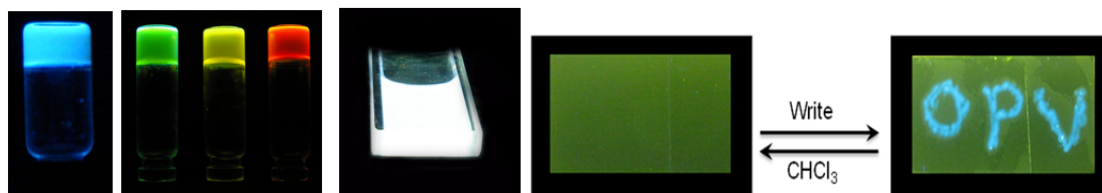
발표종류: 심포지엄, 발표일시: 금 14:40, 좌장: 이희승

Fluorescent π -Gelators and Their Application

Ayyappanpillai Ajavaghosh

National Institute for Interdisciplinary Science and Technology (NIIST), India

Self-assembly of linear π -systems is important in the field of advanced materials for optoelectronic applications. During self-assembly, the electronic interaction within these molecules induces significant changes in the properties such as absorption, fluorescence and electronic conductivity. For the past several years we have been investigating the self-assembly of oligo(p-phenylenevinylene)s (OPVs), resulting in the formation of organogels comprising of diverse morphological features. As a result, significant shift in the emission occurs towards the long wavelength region. This shift in the emission is attributed to the facile excitation energy migration within the self-assembled aggregates of different HOMO-LUMO levels as revealed by the time resolved emission studies and wavelength dependent fluorescence decay profiles. Through functional group modification and control of supramolecular interaction, we were able to tune the emission of a variety of molecular self-assemblies leading to organogels that emit at different wavelengths. Encapsulation of different acceptor molecules into the self-assembled nanostructures resulted in energy transfer in a controlled fashion resulting in emission from the acceptors. Thus, we were able prepared an organogel with white light emission. Entrapment of the gelator in a styrene gel and the subsequent polymerization resulted in a green emitting polystyrene film the fluorescence of which changed to blue upon heating. Exposure of the blue film to chloroform vapors allowed the regeneration of the green emission. This phenomenon has been used to create erasable images which are visible only upon excitation with a suitable light source. Results of these studies will be presented.



일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: **ORGN2-3**

발표분야: International Symposium on Organic Chemistry (2) : Recent Developments on Organic Functional Materials

발표종류: 심포지엄, 발표일시: 금 15:10, 좌장: 이희승

Molecular engineering of folded nanoarchitectures

Ivan Huc

University of Bordeaux - CNRS, France

Our group has developed helical foldamers – oligomers that adopt stable helical folded conformations – derived from aromatic amino acids. Some of these folded objects display unprecedented conformational stability, and constitute convenient building blocks to elaborate synthetic, very large (protein-sized) folded architectures [1]. They possess a high propensity to assemble into double, triple and quadruple helices [2]. Cavities can be designed within such synthetic molecules that enable them to act as artificial receptors [3] including for chiral guests. Water soluble analogues of these foldamers show promise in nucleic acid recognition [4].

일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: ORGN2-4

발표분야: International Symposium on Organic Chemistry (2) : Recent Developments on Organic Functional Materials

발표종류: 심포지엄, 발표일시: 금 15:55, 좌장: 윤주영

Stimuli-Responsive Nanofibers with Supramolecular Chirality

이명수

서울대 화학과

Supramolecular events take place through self-assembly process in which molecular modules spontaneously form ordered aggregates through various types of intermolecular interactions. Therefore, a major challenging task in supramolecular chemistry is the design of simple molecular components that are capable of organizing into well-defined nanostructures with tunable properties. Among many self-assembling systems, aromatic rigid building blocks have proven to be particularly interesting due to their great potentials to construct intelligent nanofibers. We have shown that rod amphiphiles with chiral side groups self-assemble into well-defined nanofibers with tunable supramolecular chirality. We have also shown that coordination polymers can adopt helical fibers with dynamic mechanical motion triggered by temperature. In this talk, our progress to exploit smart nanofibers with supramolecular chirality will be presented together with their practical implications.

일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: ORGN2-5

발표분야: International Symposium on Organic Chemistry (2) : Recent Developments on Organic Functional Materials

발표종류: 심포지엄, 발표일시: 금 16:20, 좌장: 윤주영

Foldamer Architectures with Unprecedented 3D Shapes

이희승

KAIST 화학과

In the past, enormous efforts have been devoted to mimicking the self-assembly process, but the level of control in laboratory lags behind those of the diversity and periodicity of natural system.^[1] Thus, it is necessary to find a suitable model system by which the relationship between a component and its resulting shapes through self-assembly could be studied systematically. In this context, β -peptide foldamers (oligomers of β -amino acids) are an excellent candidate as a model system that meets the minimum requirement – rigidity and predictability - because they adopt rigid and predictable secondary structures in solution. We have recently demonstrated that a β -peptide (an artificial protein fragment) with specific folding propensity self-assembled to form three dimensional molecular architectures with unprecedented shapes.^[2] Analysis of the powder diffraction pattern of the assemblage provided a new insight into the detailed molecular arrangement.^[3] References:[1] Han, T. H.; Ok, T.; Kim, J.; Shin, D. O.; Ihee, H.; Lee, H.-S.*; Kim, S. O.* *Small* 2010, 6, 945.[2] Kwon, S.; Jeon, A.; Yoo, S. H.; Chung, I. S.; Lee, H.-S.* *Angew. Chem. Int. Ed.* 2010, 49, 8232.[3] Kwon, S.; Shin, H. S.; Gong, J.; Eom, J.; Jeon, A.; Chung, I. S.; Cho, S. J.*; Lee, H.-S.*, *submitted*.

일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: ORGN2-6

발표분야: International Symposium on Organic Chemistry (2) : Recent Developments on Organic Functional Materials

발표종류: 심포지엄, 발표일시: 금 16:45, 좌장: 윤주영

Biomedical applications of photofunctional dendrimer

장우동

연세대 화학과

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

일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: **MEDI-1**

발표분야: Current Trend and Future in Cardio Vascular Disease

발표종류: 심포지엄, 발표일시: 목 14:00, 좌장: 남기엽

Roles of Two Major Tyrosine Kinase Receptors- VEGFR2 and Tie2 in Tumor Angiogenesis

고규영

KAIST 의과대학원

Two major tyrosine kinase receptors ? VEGFR2 and Tie2 are mainly expressed in blood endothelial cells and promote angiogenesis during embryonic development and pathologic processes including tumor. Five VEGFR ligands have been identified: VEGF-A, VEGF-B, VEGF-C, VEGF-D and placental growth factor (PlGF). VEGF-A interacts with both VEGFR-1 and VEGFR-2 to mediate angiogenesis, whereas VEGF-B and PlGF have high affinity to VEGFR-1 but do not promote angiogenesis. VEGF-C and VEGF-D bind to both VEGFR-2 and VEGFR-3 to promote angiogenesis and lymphangiogenesis. Various strategies for inhibiting the VEGF-VEGFR signaling pathways have been investigated over the last decade. These include neutralizing antibodies to VEGF-VEGFR, low-molecular- weight VEGFR tyrosine kinase inhibitors (e.g. sunitinib) and soluble VEGFR1 constructs (e.g., VEGF-Trap). These reagents are currently used to inhibit tumor angiogenesis for patients with various cancers. However, resistance and tumor invasion to these drugs are serious problems in the oncology clinic. Moreover, no biomarker for these drugs is currently available. Two Tie receptors have been identified: Tie1 and Tie2. No specific ligand to Tie1 has been identified. In comparison, angiopoietins are potent and selective protein molecules targeted to mainly Tie2. Angiopoietins include four proteins: Ang-1, -2, -3, and -4. Traditionally, Ang-1 and Ang4 act as agonists to Tie2, whereas Ang2 and Ang3 act as antagonists to Tie2. However, recent accumulating evidences indicate that Ang2 and Ang3 also act as agonists to Tie2 in a context-dependent manner. Various strategies for inhibiting angiopoietins-Tie2 signaling pathways have been developed over the last decade. These include anti-Ang2 antibody, antagonistic peptibody of Ang2, soluble Tie2-Fc and double anti-angiogenic protein (DAAP). These reagents are currently testing to inhibit tumor angiogenesis in the preclinical animal models.

일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: **MEDI-2**

발표분야: Current Trend and Future in Cardio Vascular Disease

발표종류: 심포지엄, 발표일시: 목 14:40, 좌장: 남기엽

Assay Development for the Urotensin Receptor Research & Drug Discovery

이승호

상명대 의생명공학과

Urotensin II (UII) is a somatostatin like cyclic peptide that has been found to have potent vasoconstrictor actions in some vascular beds of various animal species and humans. The UII system has been found to be up-regulated within the heart of patients with chronic heart failure (CHF) along with the elevation of plasma levels of UII. These observations raised the possibility that UII may be contributory to CHF disease progression, and generated a great deal of interest by pharmaceutical companies as UII receptor (UT) antagonists may have potential therapeutic benefits in the treatment of cardiac remodeling and increased peripheral vascular tone resulted from the CHF condition. This presentation will be focused on the development of the cell based HTS assay for UT antagonists as one of G protein coupled receptor (GPCR) research technologies for the receptor-ligand interaction with physiological relevances, especially the application of cell based functional assay systems as a high-fidelity screening program to reinforce the current HTS campaigns for various drug discovery programs. To develop a sensitive and reproducible assay system for UT, the luminescence based calcium mobilization assay (CMA) with a photoprotein, aequorin, was tested and validated. In addition to the UT-CMA, the Tag-lite assay platform was tested with fluo-ligand as an ongoing trial for the development of non-radiolabel binding assay. The UT-CMA assay presented reasonable Z' factors with high signal-to-noise ratio comparing to the fluorescence based UT-CMA assay and the known standard agonists/antagonists exhibited an excellent correlation with published data.

일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: **MEDI-3**

발표분야: Current Trend and Future in Cardio Vascular Disease

발표종류: 심포지엄, 발표일시: 목 15:10, 좌장: 남기엽

ACAT and DGAT Inhibitors in Neutral Lipid Metabolism

최용석

고려대 생명과학대학

Cholesterol ester (CE) and triglyceride (TG) are major forms of stored energy for many cellular functions in eukaryotes and synthesized primarily by acyl-CoA: cholesterol acyltransferase (ACAT) and acyl CoA : diacylglycerol acyltransferase (DGAT) that catalyze the final and the only committed steps in the biosynthesis pathways of CE and TG, respectively. Accumulation of CE in arteries and TG in adipose tissue are linked to major disease pathologies such as atherosclerosis, type 2 diabetes, obesity, hyperlipidemia, and fatty liver disease characterized in metabolic syndrome. Therefore, intensive efforts have been focused on the discovery of novel inhibitors targeting ACAT and DGAT for the treatment of metabolic diseases. Herein, novel ACAT and DGAT inhibitors and their biological implication will be discussed.

일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: **MEDI-4**

발표분야: Current Trend and Future in Cardio Vascular Disease

발표종류: 심포지엄, 발표일시: 목 16:00, 좌장: 안진희

Discovery of Novel Anti-ischemic Drug Candidates

이규양

한국화학연구원 신물질연구본부

Cardiovascular disease is the serious leading causes of human death worldwide. Ischemic disease comprises the largest fraction of this. Ischemia is defined as inadequate blood flow to the tissues in which oxygen supply does not meet the metabolic demands of the tissue. Despite much investigative efforts, no effective therapy has been adopted clinically for the protection of ischemia/reperfusion injury. During the last several years, we have focussed on the discovery and development of anti-ischemic drug candidates. In this presentation, our efforts are described for the discovery of anti-ischemic agents in several drug targets such as ATP-sensitive potassium channel opener, sodium/hydrogen exchanger-1 inhibitor, and poly(ADP-ribose) polymerase(PARP) inhibitor.

일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: **MEDI-5**

발표분야: Current Trend and Future in Cardio Vascular Disease

발표종류: 심포지엄, 발표일시: 목 16:40, 좌장: 안진희

Development of GCC-4401C as a promising anticoagulant

이진화

(주)녹십자 종합연구소

An anticoagulant is a substance that stops blood from clotting. A group of pharmaceuticals called anticoagulants can be used in vivo as a medication for thrombotic disorders. This prevents deep vein thrombosis, myocardial infarction and stroke. Currently, warfarin is the most widely prescribed anticoagulant drug in North America, although treatment with warfarin has several shortcomings including nonspecific interaction with many commonly used medications and even foods. As an injectable anticoagulant, heparin and low molecular derivatives are used, but they also have a serious side-effect such as heparin-induced thrombocytopenia (HIT). Recently, Factor Xa has been a notable focus directed at novel antithrombotics because of its unique position in the coagulation cascade. Factor Xa inhibition is considered to be an optimal approach to achieve strong efficacy and good safety compared to current therapies. The most advanced FXa inhibitor is rivaroxaban being developed by Bayer. Rivaroxaban has been approved in the EU and other countries for the treatment of venous thromboembolism (VTE) in patients undergoing total hip or total knee replacement surgery, but not in US. Currently, GCC is developing a novel FXa inhibitor which has demonstrated arguably advantageous developability characteristics over rivaroxaban so far. Herein, we wish to discuss development of GCC-4401C toward a novel promising anticoagulant.

일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: **MEDI-6**

발표분야: Current Trend and Future in Cardio Vascular Disease

발표종류: 심포지엄, 발표일시: 목 17:20, 좌장: 안진희

최초 국내개발 고혈압 치료제 카나브

김지한

보령제약(주) 중앙연구소

2010년 9월 신약허가를 득한 고혈압 치료제 카나브(물질명 : 피마살탄)는 국내 최초의 ARB 로써 기존 고혈압치료제인 로잘탄에 비해 독성은 낮추고 효력은 극대화시킨 신약이다. 피마살탄은 최초의 ARB 고혈압 치료제인 로잘탄의 이미다졸 유도체 대신에 새로운 헤테로 방향족 화합물을 도입하였고, 약 700 종의 화합물을 제조하였다. 그 중 6-membered ring 인 pyrimidine 모핵을 가지는 새로운 pyrimidinone 유도체를 Lead 화합물로 도출하였다. 도출된 Lead 화합물의 짧은 작용시간을 극복하기 위해 Lead Optimization 을 통해 최종 화합물을 도출하였다. 다양한 동물모델에서의 효력을 확인하였으며, 국내외 전문기관을 통해 일반독성, 유전독성, 안전성약리, 발암성 독성 등을 확인하였다. 영국에서의 1 상 임상시험을 근거로 안전영역을 마련하여 서울대 임상의학연구소의 한국 환자들에서 2 상 임상시험을 시작으로 전국 24 개 병원에서 3 상 임상시험과 제형 비교 임상, 약물상호작용 등의 서브 스터디를 거치면서 적정용량은 물론 한국 환자에서의 다양한 특성에 대한 자료들을 확보하였다. 현재 보령에서는 국외 라이선스 아웃을 목표로 다양한 활동을 하고 있으며, 피마살탄의 복합제 개발로 제품력을 극대화 하기 위해 다수의 비임상, 임상 시험들을 진행하고 있다.

일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: MAT1-8

발표분야: Chemistry in Medical Materials

발표종류: 분과기념강연, 발표일시: 목 17:00, 좌장: 허남희

Nanomorphic Zeolitic Architectures Built by Zeolite-Structure-Directing Surfactant for Active and Long-Lived Catalytic Applications

유훈

KAIST 화학과

Generation of nanomorphic architectures having larger pores with microporous zeolite crystallinity is a great challenge in modern catalytic science and technology because such materials are expected to have high catalytic functions and selectivity. In this lecture, we focus on a synthetic strategy for the generation of nanomorphic zeolitic materials built with ultrathin frameworks of single-unit-cell thickness or even less. The strategy uses a surfactant molecule that possesses a zeolite-structure-directing functional group while the surfactant tails are organized to generate nanostructured architectures. The present strategy using a portion of molecule shows a striking difference from conventional zeolite structure-directing methods that use the entire part of small organic molecule. Depending on the detailed synthetic conditions, the surfactant molecules can generate a random assembly of 2-nm thick nanosheets, regular stacking of multilamellar nanosheets, nanospongy-like disordered network of nanocrystals, and other various types of hierarchically porous architectures. The large number of acid sites on the external surface of these materials renders them highly active for the catalytic conversion of large organic molecules, and the reduced crystal thickness facilitates diffusion and thereby dramatically suppresses catalyst deactivation through cokes deposition during reactions. It is expected that the present synthesis approach could be applied to various types of zeolites to improve their performance in a range of important catalytic applications such as the production of renewable energy and the development of green chemical processes.

일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: **MAT1-1**

발표분야: Chemistry in Medical Materials

발표종류: 심포지엄, 발표일시: 목 13:30, 좌장: 천진우

Science and Technology of Semiconductor Quantum Dots: The Importance of Excitons

Moungi Bawendi

Massachusetts Institute of Technology, U.S.A.

Semiconductor nanocrystals are the prototypical nanomaterial with well developed size dependent electronic properties. Probing and understanding the size dependent properties of the excitons initially motivated much of the research in their chemistry and physics. More recently, applications ranging from biomedical imaging to displays and solar energy conversion have renewed the need for both a thorough chemical understanding of nanocrystal design and of their physical properties. This talk will review two topics: (1) Progress in the chemistry and physics of nanocrystal quantum dots in the context of their recent applications in biomedical imaging, light emission and solar energy conversion, and (2) Recent advances in the spectroscopic characterization of these materials at the level of single nanocrystals.

일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: **MAT1-2**

발표분야: Chemistry in Medical Materials

발표종류: 심포지엄, 발표일시: 목 14:15, 좌장: 이해신

Mussel Derived Adhesives for Bio-medical Applications

박태관

KAIST 생명과학과

Herein, we present mussel-inspired adhesives for various bio-medical applications including tissue adhesives, medical imaging, and treatment of cardiovascular diseases. Blue marine mussel (*Mytilus edulis*) secretes adhesive proteins containing an unusual amino acid, L-3,4-dihydroxy-L-phenylalanine (DOPA), which is particularly abundant in the interface between adhesive pads and opposing surfaces. For tissue adhesives, hyaluronic acid (HA) conjugated with dopamine (HA-DN) was reacted with thiol end-capped Pluronic F127 copolymer (Plu-SH) to produce a lightly cross-linked HA/Pluronic composite gel structure based on Michael-type catechol-thiol addition reactions. Adhesion study using subcutaneous tissue of mouse revealed that the hydrogels showed excellent tissue-adhesion properties. Mussel-inspired adhesion could also be utilized as a surface coating strategy for the functionalization of metallic stent and polymeric balloon catheter. For the surface immobilization of heparin on the surface of cobalt-chromium alloy (L605) stent, dopamine-derivatized heparin was synthesized and anchored on the surface. A PTX eluting multilayer composed of anionic HA-g-PLGA micelles, heparin, and PLL was self-assembled on the metal surface by a layer-by-layer fashion. The proliferation of human coronary artery smooth muscle cells was successfully arrested by controlled released PTX from the therapeutic multilayer coated on the metallic substrate. We also demonstrate immobilization of heparin on the balloon surface and layer-by-layer assembly of PTX-loaded albumin nanoparticles and heparin for drug eluting balloon (DEB).

일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: **MAT1-3**

발표분야: Chemistry in Medical Materials

발표종류: 심포지엄, 발표일시: 목 14:45, 좌장: 이해신

Cell-interactive scaffolds for tissue engineering applications

신흥수

한양대 생명공학과

The central strategy in tissue engineering involves a biomaterial scaffold as a delivery carrier of cells and a depot to deliver bioactive molecules. The ability of scaffolds to control cellular response to direct particular repair and regeneration processes is essential to obtain functional tissue engineering constructs. Therefore, many efforts have been made to understand local interactions of cells with their extracellular matrix (ECM) microenvironment and exploit these interactions for designing an ideal scaffold mimicking the chemical, physiological, and structural features of native ECM. ECM is composed of a number of biomacromolecules including proteins, glycosaminoglycans, and proteoglycans, which are assembled together to form complex 3-dimensional network. Cells are bound to these ECM components, which in many cases, is implicated in critical cell fate process such as adhesion, proliferation, differentiation, and survival. In this presentation, our approaches to develop cell-interactive scaffolds for modulation of cell function by providing several exemplary works of engineering bone, muscle, ischemic, and neural tissue.

일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: MAT1-4

발표분야: Chemistry in Medical Materials

발표종류: 심포지엄, 발표일시: 목 15:10, 좌장: 이해신

Effective sensitization of drug-resistant colorectal cancer cells by new cationic micelle-based combined delivery of anticancer drug and siRNA

정지훈

성균관대 약학과

Chemotherapy is still the most widely used approaches for cancer treatment. One of the most challenging factors of chemotherapy is to overcome intrinsic and acquired drug resistance of cancer cells. Majority of anticancer drugs depend mainly on the induction of apoptosis for cancer cell death. However, since expression of antiapoptotic proteins such as Bcl-2 and inhibitors of apoptosis (IAPs) is significantly elevated in many types of cancers, the efficiency of chemotherapy is often limited by the resistance mechanism developed by cancer cells. In addition, the treatment of anticancer drugs can also induce the expression of the drug-resistant proteins. Simultaneous use of apoptosis-inducing drug and an inhibitor that blocks the action of anti-apoptotic proteins would address the drug resistance problems for cancers. In this case, best results can be expected if an apoptosis-inducing anticancer drug and inhibitors for anti-apoptotic proteins exist in the same space and time, i.e., the same intracellular space. In this study, we synthesized new cationic micelle having controlled amphiphilicity and used as a carrier for combined delivery of water-insoluble anticancer drug and nucleic acid drug. The combined delivery system demonstrated a desired synergic effect in an animal model bearing tumor xenograft.

일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: MAT1-5

발표분야: Chemistry in Medical Materials

발표종류: 심포지엄, 발표일시: 목 15:45, 좌장: 정지훈

In situ Gelled Polypeptide Hydrogel Scaffolds for Tissue Engineering and Regenerative Medicine

임동우

한양대 생명나노공학과

In situ gelled polypeptide hydrogel scaffolds have been of great interest as injectable biomaterials for tissue repair, defect filling for tissue reconstitution and controlled drug release reservoirs because they are rapidly formed in vivo by physical- or chemical crosslinking means, and they provide encapsulated cells with the artificial extracellular matrices (ECMs) which are composed of polypeptides derived from native ECMs in tissues. Specifically, polypeptides with environmental stimuli-responsiveness are self-assembled by controlling temperature, pH, or ionic strength while polypeptides with reactive functional groups are in situ chemically crosslinked. We have been developing stimuli-responsive elastin-like polypeptides (ELPs) by genetic- and protein engineering. Genetically-encoded ELPs exhibit lower critical solution temperature (LCST) transition behavior; they are soluble at temperatures below their LCST and become insoluble at temperatures above it. With environmental responsiveness of ELPs, we recently reported temperature-triggered, physically crosslinked ELP block copolymer hydrogel scaffolds as well as in situ chemically crosslinked ELP hydrogel scaffolds for drug delivery, tissue engineering and regenerative medicine. Especially, rheological- and mechanical- properties of the physically crosslinked ELP block copolymer hydrogels were largely controlled by the amino acid sequence, length and charged state of the hydrophobic block, and salt concentration. It suggests that their load-bearing properties could be finely tuned by rationally designed ELP blocks and optimized ionic strength under physiological conditions. Special emphasis will be also given to rapid crosslinking of the ELP block copolymers with hydroxymethylphosphines for minimally invasive in vivo implantation of tissue engineering scaffolds. This study opens a new avenue to develop a new class of biomimetic tissue engineering scaffolds as injectable biomaterials.

일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: **MAT1-6**

발표분야: Chemistry in Medical Materials

발표종류: 심포지엄, 발표일시: 목 16:10, 좌장: 정지훈

Anti-Viral RNAi Therapeutics with Lipid-Like Nanoparticles

조승우

연세대 생명공학과

Delivery of small interfering RNA (siRNA) is an emerging approach of treating viral diseases. In this study, we report the use of lipid-like synthetic molecules, named lipidoids, as siRNA carriers for treatment of hepatitis C virus (HCV) that causes chronic hepatitis and liver cirrhosis. The lipidoids were synthesized by conjugation addition of molecules with long alkyl-chains to amines. Delivery of siRNA with lipidoids significantly reduced the expression of a target enzyme which is required for HCV replication in human hepatic cells. Accordingly, HCV replication in HCV-infected human hepatic cells was suppressed by lipidoid-mediated siRNA delivery. Lipidoids developed in this study may be useful for *in vivo* delivery of anti-viral RNAi therapeutics.

일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: **MAT1-7**

발표분야: Chemistry in Medical Materials

발표종류: 심포지엄, 발표일시: 목 16:35, 좌장: 정지훈

Molecularly Engineered Cell Engineering

이동윤

한양대 생명공학과

Insulin-secreting pancreatic islet transplantation is one of the most promising strategies for patients suffering from diabetes mellitus, but they must be eliminated by host's immune graft rejection. To protect transplanted islets in host, bioengineered pancreatic islets are being developed. To this end, surface modification with biocompatible polymer and cellular reconstruction technology are introduced. Here PEG-based chemical immunoprotection can provide an effective therapy that protects transplanted islets at least for one year when CsA was administered. Also, when the size of pancreatic islets was reconstructed with bio-MEMS technology, the viability and functionality of islet cell cluster could be improved. Finally, these bioengineered pancreatic islets could be tracked in vivo through islet labeling with MRI contrast agent. Therefore, these technologies could strongly support the successful pancreatic islet transplantation for hunting diabetes mellitus.

일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: **MAT2-1**

발표분야: Emerging Photonic Nanomaterials

발표종류: 심포지엄, 발표일시: 금 13:30, 좌장: 남좌민

Assembly of Biomimetic Peptoid Polymers

남기태

서울대 재료공학부

The design and synthesis of protein-like polymers is a fundamental challenge in materials science. A biomimetic approach is to explore the impact of monomer sequence on non-natural polymer structure and function. We present the aqueous self-assembly of two peptoid polymers into extremely thin two-dimensional (2D) crystalline sheets directed by periodic amphiphilicity, electrostatic recognition and aromatic interactions. Peptoids are sequence-specific, oligo-N-substituted glycine polymers designed to mimic the structure and functionality of proteins. Mixing a 1:1 ratio of two oppositely charged peptoid 36mers of a specific sequence in aqueous solution results in the formation of giant, free-floating sheets with only 2.7 nm thickness. Direct visualization of aligned individual peptoid chains in the sheet structure was achieved using aberration-corrected transmission electron microscopy. Specific binding of a protein to ligand-functionalized sheets was also demonstrated. The synthetic flexibility and biocompatibility of peptoids provide a flexible and robust platform for integrating functionality into defined 2D nanostructures. In the later part of my talk, we describe the use of metal ions to construct two-dimensional hybrid films that have the ability to self-heal. Incubation of biomimetic peptoid polymers with specific divalent metal ions results in the spontaneous formation of uniform multilayers at the air-water interface. We anticipate that ease of synthesis and transfer of these two-dimensional materials may have many potential applications in catalysis, gas storage and sensing, optics, nanomaterial synthesis, and environmentally responsive scaffolds.

일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: **MAT2-2**

발표분야: Emerging Photonic Nanomaterials

발표종류: 심포지엄, 발표일시: 금 14:00, 좌장: 남좌민

Synthesis and Thermodynamically Controlled Anisotropic Assembly of DNA-Silver Nanoprism Conjugates for Diagnostic Applications

이재승

고려대 신소재공학부

We have synthesized DNA-silver nanoprism conjugates using the thiol-silver interaction and have assembled them into anisotropic structures with distinctive optical properties simply by controlling thermodynamic conditions. The reversible assembly formation takes advantage of the natural anisotropic architecture of the silver nanoprisms and the cooperative properties of their DNA conjugates. The anisotropic assemblies have been observed not only ex situ by TEM but also in situ in a solution by UV-vis spectroscopy. We have further investigated biodiagnostic applications of the DNA-silver nanoprism conjugates for the colorimetric and quantitative detection of DNA with high selectivity and sensitivity in the full visible range based upon their unique distant-dependent optical properties.

일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: **MAT2-3**

발표분야: Emerging Photonic Nanomaterials

발표종류: 심포지엄, 발표일시: 금 14:30, 좌장: 남좌민

Live-Cell Imaging with Lanthanide Ion-Doped Upconverting Nanoparticles

이강택

한국화학연구원 나노바이오융합연구센터

Lanthanide ion-doped upconverting nanoparticles (UCNPs), which emit visible photons upon NIR excitation, have recently been recognized as promising biological imaging probes thanks to their unique optical properties. The luminescence of UCNPs was monitored at the single-particle level using a sensitive wide-field fluorescence microscope system equipped with a 980-nm diode laser and an EMCCD camera. It was found that single UCNPs exhibit neither photoblinking on the millisecond time scale nor photobleaching even under long-time continuous illumination. We also observed that the hydrophilic and biocompatible surface coating led to efficient uptake of UCNPs by cells. Owing to the NIR excitation, the luminescence images were free of autofluorescent background from cellular environment and the cell samples were not significantly damaged. We took advantage of both the photostability of UCNPs and the noninvasiveness of NIR excitation to investigate intracellular transport of nanoparticles in live cells. The UCNPs incubated with live HeLa cells were internalized through endocytosis and transported to the perinuclear region. We found that the accumulation of particles was followed by the significant signal loss, presumably due to exocytosis. In particular, we visualized, in real time, the active transport of UCNPs operated by motor proteins along the microtubules.

일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: **MAT2-4**

발표분야: Emerging Photonic Nanomaterials

발표종류: 심포지엄, 발표일시: 금 15:15, 좌장: 한상우

Plasmonic Nanomaterials for smSERS(single molecule Surface-Enhanced Raman Scattering)

서영덕

한국화학연구원 나노바이오융합 연구센터

Since smSERS was independently reported by S. Nie group and K. Kneipp group in 1997, tremendous amount of interest has been shown to this field because Raman spectroscopy can provide molecular fingerprint together with multiplexing capability in bioassay. Regarding to the origin of this smSERS phenomena, so called “SERS hot spot”, these two groups argued against each other for several years: Nie group argued sharp edge in nanostructure, such as corners of a silver nanorod or even of a single nanoparticle, can play as a hot spot of smSERS, while Kneipp group argued they could observe smSERS signal only from colloidal aggregation in solution. Later on, Brus group and others showed that SERS hot spots, formed at the junction of two nanoparticles, likely play a major role in smSERS. However, formation of these smSERS-active nanostructures, mostly dimer or colloidal aggregation of Ag or Au nanoparticles adsorbed with Raman active molecules (e.g., Rhodamine 6G), is a random process driven by salt-induced non-specific aggregation. This fact has been a main hurdle for smSERS toward advanced applications. Based on the idea that controlling this nano gap between two noble metal nanoparticles is the key to realize reliable smSERS, we have designed a gold-silver nano dumbbell (GSND). Two gold nano particles with different sizes were linked to each other by double helix DNA (30mer), with a single Raman dye molecule labeled at the center position, to fix the two at a known gap distance (~10 nm). Then we narrowed the gap down to < 1 nm by standard silver staining method to endow the GSND with single molecule sensitivity. We have successfully detected smSERS signals, as well as typical single molecular blinking and polarization behaviors, from each GSNDs by Nano Raman spectroscopy at the single particle level.

일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: **MAT2-5**

발표분야: Emerging Photonic Nanomaterials

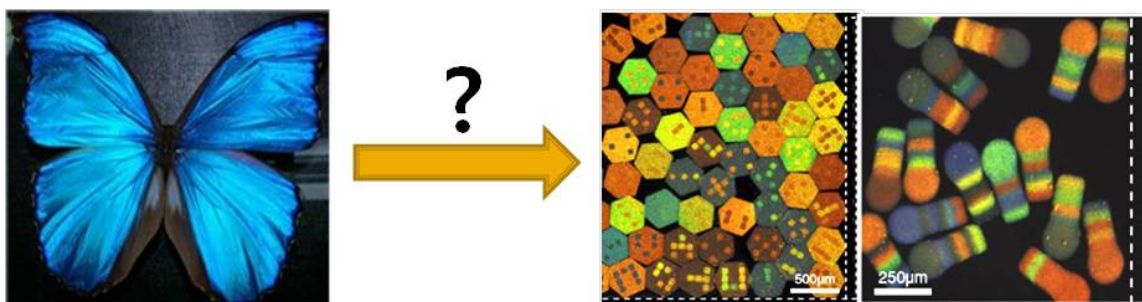
발표종류: 심포지엄, 발표일시: 금 15:45, 좌장: 한상우

강자성나노입자의 자기조립을 이용한 컬러바코드 마이크로입자와 그 응용 (Color Barcoded Microparticles using Magnetic Self- Assembly of Superparamagnetic Nano Particle Cluster)

권성훈

서울대 전기공학부

Encoded particles have a demonstrated value for multiplexed high-throughput bioassays such as drug discovery and clinical diagnostics. In diverse samples, the ability to use a large number of distinct identification codes on assay particles is important to increase throughput. Proper handling schemes are also needed to readout these codes on free-floating probe microparticles. Colored beads are widely used as encoded particles but their coding capacity is practically limited to the thousands and the fabrication of those particles requires precise mixing of multiple coloring materials. In this talk, we present vivid, free-floating structural coloured particles with multi-axis rotational control using a colour-tunable magnetic material and a new printing method. Instead of using multiple coloring materials, we have used a single structural and coloring material named 'M-Ink' to the fabricate color barcoded microparticles. Our colour-barcoded magnetic microparticles offer a coding capacity easily into the billions with distinct magnetic handling capabilities including active positioning for code readouts and active stirring for improved reaction kinetics in microscale environments. A DNA hybridization assay is done using the colour-barcoded magnetic microparticles to demonstrate multiplexing capabilities and it is proven that the spinning motion of the particle reduces incubation time of the DNA binding assay by an order of magnitude.



일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: **ELEC1-1**

발표분야: Nanoelectrochemistry I: Electrocatalytic Nanomaterials

발표종류: 심포지엄, 발표일시: 목 14:00, 좌장: 김주훈

Electrocatalysis of Glucose and Oxygen at Nanostructured Gold Surfaces: Structure Dependent Electrocatalysis and Its Application

김종원

충북대 화학과

Electrooxidation of glucose and electroreduction of oxygen are investigated at nanostructured gold surfaces. In the first part of this presentation, nanoporous gold (NPG) with controlled surface structures by applying different deposition charges during the formation of Ag-Au layers is utilized. As the deposition charge increases, the NPG surfaces exhibit smaller ligament/pore structures and the electrocatalytic oxidation of glucose becomes more effective. Voltammetric responses of NPG suggest that the electrocatalytic oxidation arises from the enrichment of (110) or (100) surface orientation of gold with higher deposition charges. The electrooxidation of glucose is retained at NPG surfaces with higher deposition charges in the presence of Cl^- , which suggests possible applications to the amperometric glucose detection in biological samples. In the second part, the formation of nanoplate gold and dendritic gold rod structures via simple electrodeposition and their electrocatalysis are presented. The surface structures are regulated by applying different deposition potentials. The correlation between surface nanostructures and electrocatalytic activities is examined by electrochemical methods and possible mechanisms are discussed.

일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: **ELEC1-2**

발표분야: Nanoelectrochemistry I: Electrocatalytic Nanomaterials

발표종류: 심포지엄, 발표일시: 목 14:30, 좌장: 김주훈

Electrochemical Study of Adsorption Kinetics of Thin Organic Layer

황성필, 계주홍

명지대 화학과

Self-assembled monolayers (SAMs) on gold surface via thiol-sulfur bond have attracted considerable interest nowadays owing to their significant role in nanotechnology and the variety of their potential applications by the tailored physical and chemical properties of interface. The synthetic accessibility of organic adsorbate enables easy anchor of various complex molecules so that the number of newly synthesized compounds for SAMs are getting increase. Although the adsorption kinetics of SAMs depend on various factors such as concentration of adsorbate, temperature, and chemical structure of adsorbates, the adsorption kinetics of each adsorbate still remains largely uncharacterized especially for solution-phase assembly because in-situ or ex-situ techniques including ellipsometry, scanning tunneling microscopy (STM), atomic force microscopy (AFM), quartz crystal microbalance, second harmonic generation (SHG), surface plasmon resonance (SPR), and electrochemistry requires a expensive setup and has the limited resolution in time. In this presentation, the simple and affordable experimental technique for the adsorption kinetics in the solution phase based on the electrochemistry will be presented. The obtained results are in good accordance with the previously reported one found by other technique demonstrating that our simple method is a valuable technique for the characterization of the adsorption kinetics.

일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: **ELEC1-3**

발표분야: Nanoelectrochemistry I: Electrocatalytic Nanomaterials

발표종류: 심포지엄, 발표일시: 목 15:00, 좌장: 김주훈

Improvement of Metal Catalytic Activity toward Electrochemical Reactions

이영미

이화여대 자연과학대학/화학전공

The electrocatalytic activity of the metals is of great interest, particularly in the field of fuel cells and electrochemical sensors since the activity correlates directly with the device efficiency. To improve the metal catalytic activity, increasing the surface area using nanoparticles, nanoporous structures; and modification with second metals have been employed commonly. In this presentation, we demonstrate the improvement of novel metal electrocatalytic activity by the electrochemical treatment and size/morphology control. Indeed, the activity of platinum, gold, and palladium was examined before and after the pretreatment or morphology control toward electrochemical reactions such as oxygen reduction, hydrogen peroxide reduction/oxidation which are important in the area of fuel cells and enzyme-based sensors.

일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: **ELEC1-4**

발표분야: Nanoelectrochemistry I: Electrocatalytic Nanomaterials

발표종류: 심포지엄, 발표일시: 목 15:50, 좌장: 김종원

Modification of Carbon-based Electrodes with Dendrimer-encapsulated Nanoparticles

김주훈

경희대 화학과

Amine-terminated poly(amidoamine) dendrimers were immobilized on glassy carbon electrodes (GCEs) via electrochemical oxidation of the terminal amine groups of dendrimers. The electrochemical immobilization of dendrimers was confirmed by cyclic voltammetry and X-ray photoelectron spectroscopy. The immobilized dendrimer films were robust and behaved as charge-selective electrochemical gates for oppositely charged redox molecules, i.e. $\text{Ru}(\text{NH}_3)_6^{3+}$ and $\text{Fe}(\text{CN})_6^{3-}$. The immobilization approach was applied to assemble dendrimer-encapsulated nanoparticles (DENs) on GCEs, and the resulting DEN films show high electrocatalytic properties.

일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: **ELEC1-5**

발표분야: Nanoelectrochemistry I: Electrocatalytic Nanomaterials

발표종류: 심포지엄, 발표일시: 목 16:20, 좌장: 김종원

Enhancement of the Electrocatalytic Activities of Au Nanoparticles and Their Decrease with Aging

양해식

부산대 화학과

Much effort has been devoted to achieving high activities via morphology or composition control and/or via thermal, cathodic, or chemical treatment. Nevertheless, the dependence of electrocatalytic activities on aging has never been investigated. If electrocatalytic activities of nanomaterials change with aging, the activities measured just after their preparation do not represent normal ones. The electrocatalytic activities of Au nanoparticles toward the electrooxidation of H_2O_2 , glucose, and formic acid are enhanced by NaBH_4 treatment (dipping electrodes in NaBH_4 solution), cathodic treatment (application of a potential at which hydrogen is generated electrochemically), and anodic treatment (application of a potential at which Au oxide is generated). However, the enhanced activities slowly decrease with aging. Moreover, Au nanoparticles freshly prepared by four different methods (electrodeposition; reduction of Au ions with NaBH_4 , citrate, and ascorbate, respectively) also show high electrocatalytic activities, but the activities slowly decrease with aging both in air and in solution.

일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: **ELEC2-1**

발표분야: Nanoelectrochemistry II: Electrochemical Sensors Using Nanomaterials

발표종류: 심포지엄, 발표일시: 금 09:30, 좌장: 양해식

Electrochemical Biosensors Based on Reduced Graphene Oxide

김규원, 박혜진, Al-Monsur Jiaul Haque, Md Mohibul Islam Khan

인천대 화학과

Graphene has attracted considerable attention in electrochemical applications due to its distinctive advantages, such as high electrical conductivity, large surface area, good electrocatalytic activity, and π -conjugation, over those of carbon family materials. Hydrophobic property also is important for bio-immobilization because it doesn't disturb the ordered network from the π -conjugation. In this talk, the modification of electrode surfaces with chemically or electrochemically reduced graphene oxide (RGO), and the immobilization of biomolecules as probes onto the surfaces are introduced. We demonstrate electrochemical biosensors realized on the RGO-modified electrode surfaces, which have been developed by the combination of the advantages.

일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: **ELEC2-2**

발표분야: Nanoelectrochemistry II: Electrochemical Sensors Using Nanomaterials

발표종류: 심포지엄, 발표일시: 금 10:00, 좌장: 양해식

Electrochemistry at nanoporous interface and its applications

정택동

서울대 화학부

The nanoporous electrodes, particularly mesoporous structures, provide not only a unique system to investigate the potential profile in the electric double layer but also abundant implication of potential substrates for sensory devices. Our work significantly extended the scope that had been limited within lyotropic liquid crystalline template or potential controlled self-assembly producing 1D nanopores, and suggest a new way to mass production of nanoporous metal thin films. 3D nanoporous film was electroplated from L2 phase and showed the 3D pores of 1~3 nm wide and several hundreds of high roughness factors. This new film is greatly practical for electrocatalytic applications that require fast mass transport and alleviated pore clogging. A representative example of the novel applications is the electrochemical determination of glucose concentration without using enzyme, which will lead to possible breakthroughs in achieving the enzymeless glucose sensor. Another class of its valuable applications include solid-state reference electrode and thin film-based pH sensor which can be miniaturized into a microfluidic system. Remarkable suppression of interfacial impedance at the nanoporous surfaces allows neural stimulator, extracellular recording probes, and many others. In this presentation, both detailed fundamental electrochemical behavior at nanoporous interfaces and a variety of its uses will be introduced.

일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: **ELEC2-3**

발표분야: Nanoelectrochemistry II: Electrochemical Sensors Using Nanomaterials

발표종류: 심포지엄, 발표일시: 금 10:30, 좌장: 양해식

Biosensing of Carbohydrate and Carbohydrate-Binding Proteins Based on Carbohydrate-Stabilized Gold Nanoparticles

이원용

연세대 화학과

The quartz crystal microbalance has been explored as a biosensing platform in order to study on the interactions between carbohydrates and proteins. Self-assembled monolayer of thiol-modified carbohydrates have been prepared and used for the interaction studies as well as the quantitation of carbohydrate-binding proteins. A protein, concanavalin A (Con A), from canavalia ensiformis, which binds specifically to mannoside and glucoside, was used as a model system to study the interactions between carbohydrates and proteins. The binding constants of the carbohydrates self-assembled on a gold of quartz-crystal and proteins has been determined by this approach. In order to amplify the QCM signal, mannose-stabilized gold nanoparticles have been employed. Since the Con A has four binding sites, the mannose-stabilized gold nanoparticles can be bound to the Con A, which is already bound to the carbohydrates self-assembled on the gold electrode of quartz crystal, thus increasing the QCM signal with a good detection limit of 0.19 nM Con A. In addition, a highly sensitive electrochemical lectin biosensor has been developed for using carbohydrate-stabilized gold nanoparticles and silver-enhancement technique. A target lectin protein was specifically bound to the self-assembled monolayer of thiolated mannose on a gold electrode. Mannose-stabilized gold nanoparticles were added to form a sandwich-type complex with the Con A and were followed by silver enhancement process to coat the mannose-stabilized gold nanoparticles with silver metal. The coated metallic silver was dissolved in an acidic solution and the resulting silver ions were detected by anodic stripping voltammetry. The present lectin biosensor gave a linear response for Con A concentration from 0.084 $\mu\text{g/mL}$ to 50.0 $\mu\text{g/mL}$ with a remarkable detection limit of 0.070 $\mu\text{g/mL}$.

일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: **ELEC2-4**

발표분야: Nanoelectrochemistry II: Electrochemical Sensors Using Nanomaterials

발표종류: 심포지엄, 발표일시: 금 11:15, 좌장: 정택동

Creating Multifunctional Proton Selective Nanobiosensors for Biological and Environmental Applications

이혜진

경북대 화학과

Electrochemistry at the interface between two immiscible electrolyte solutions (ITIES) has offered a superb sensing platform for the analysis of non-redox and biological species with an enhanced selectivity given by incorporating target specific ionophores into an organic electrolyte phase. In this talk, we highlight our recent advances made on the development of amperometric proton selective sensors utilizing micro-ITIES that can be powerfully applied to the fields of environmental and biological sciences. The detection methodology is based on measuring current changes associated with the proton transfer by a proton selective ligand (e.g., ETH1778) across a micro-hole interface between the water and polyvinylchloride -2-nitrophenyloctylether (PVC-NPOE) gel phase. As a first example, the selective detection of organophosphate (OP) compounds (i.e., paraoxon, parathion and methyl patathion) is demonstrated where current changes associated with protons generated by the hydrolysis of OP with the organophosphorus hydrolase (OPH) were correlated to the OP concentration. Another example is to create glucose sensing platform using the proton transfer reaction across the micro-hole ITIES followed by the glucose oxidase reaction with glucose. Both the detection methodologies were realized on a disposable strip based sensing platform created using a simple polydimethylsiloxane (PDMS) microfabrication in conjunction with a screen printed silver/silver chloride electrode preparation. Finally we will present newly developed hydrophobic ionic liquids which can replace the organic solvent and supporting electrolyte in the ITIES and their excellent performances in the ion sensing capability with nanomaterials.

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장소: 제주ICC

발표코드: **ELEC2-5**

발표분야: Nanoelectrochemistry II: Electrochemical Sensors Using Nanomaterials

발표종류: 심포지엄, 발표일시: 금 11:45, 좌장: 정택동

Electrochemical Sensing Using Quantum-Sized Gold Nanoparticles

이동일

연세대 화학과

Quantum-sized gold nanoparticles have received considerable attention recently because of their unique size-dependent electrochemical, optical and catalytic properties. While much progress has been made toward understanding their structures and fundamental properties, the technological application of such nanoparticles is still scarce. I present here the first utilization of the quantum-sized Au25 nanoparticles in electrocatalysis and electrochemical sensing. The Au25 film modified electrode exhibited excellent mediated electrocatalytic activity that was utilized for amperometric sensing of several biologically or industrially significant analytes, such as ascorbic acid, uric acid, sulfite and dopamine. The electron transfer dynamics in the Au25 film was examined as a function of Au25 concentration, which manifested the dual role of Au25 as an electronic conductor as well as a redox mediator. The electron transfer study has further revealed the correlation between the electronic conductivity of the Au25 film and the sensing sensitivity.

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장소: 제주ICC

발표코드: **ENVR1-1**

발표분야: Abiotic/biotic Interactions in Nano-interfaces

발표종류: 심포지엄, 발표일시: 금 09:00, 좌장: 이우진

Nano-Bio Catalytic Processes for Degradation of Organic Micropollutants

장윤석

포항공과대 환경공학부

Environmental pollution caused by organic micropollutants is nowadays one of the major emerging environmental concerns due to their negative effects on aquatic biota and human life. Organic micropollutants are various classes of chemicals including pesticides, pharmaceutical and personnel, and several industrial chemicals. As micropollutants are heterogeneous in nature and recalcitrant to degradation, their removal or degradation is highly influenced by their chemical structural and properties, and many of them pass through the conventional wastewater treatment process without significant change. Therefore, efficient treatment methods are necessary in order to completely remove/degrade the halogenated micropollutants from wastewater system. In this study, a strategy with a combination of sequential nano and bio catalytic processes is proposed for the degradation of selected halogenated micropollutants including personal care products and flame retardants that are ubiquitous in the environment.

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장소: 제주ICC

발표코드: ENVR1-2

발표분야: Abiotic/biotic Interactions in Nano-interfaces

발표종류: 심포지엄, 발표일시: 금 09:25, 좌장: 이우진

Compound-specific dechlorination of chlorinated hydrocarbons by nano-scale iron

송호철

세종대 환경에너지융합학과

Reduction experiments with laboratory synthesized nano-scale iron were carried out to investigate compound-specific dechlorination pattern of chlorinated hydrocarbons. The transformation of chlorinated ethenes by nano-scale iron proceeded to fully dechlorinated products (ethene and ethane), with no production of chlorinated intermediates, which were often observed in the reactions with commercial grade iron samples. The effect of chlorination on the relative reaction rate of chlorinated ethenes observed sharply contrasts to many prior studies in that it showed increasing reaction rate with decreasing chlorination of compound (vinyl chloride (VC) > dichloroethenes (DCEs) > trichloroethene (TCE) > tetrachloroethene (PCE)). This reversed trend suggests the reduction of chlorinated ethenes by nano-scale iron did not occur under thermodynamic control, but proceeded via a catalytic pathway, in which the rate of reaction was inversely proportional to the number of chlorine atoms to be removed from the molecules. On the other hand, the reduction of chlorinated ethanes showed little evidence of catalytic reactions, suggesting the reduction of haloalkanes dose not proceed via catalytic pathways, but it likely occurs via direct electron transfer from iron-associated surface to the physically adsorbed substrates. Commercial grade micro-scale iron samples did not show catalytic capability in reducing TCE, suggesting catalytic property is unique to nano-scale iron.

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장소: 제주ICC

발표코드: **ENVR1-3**

발표분야: Abiotic/biotic Interactions in Nano-interfaces

발표종류: 심포지엄, 발표일시: 금 09:50, 좌장: 이우진

Green Environmental Application of Biogenic TiO₂ Nanoparticles from Marine Diatoms

김영, *G. Rorrer, *L. Semprini, *C. Jeffryes

고려대 환경시스템공학과 *Oregon State University, U.S.A.

The UV photocatalytic activity of biogenically produced TiO₂ nanoparticles is being evaluated to determine whether it promotes transformation of chloroform (CF) via oxidation and reduction pathways. CF is a disinfection by-product formed during drinking water chlorination. We are comparing biogenically produced nanoparticles versus benchmark (non-biogenic) TiO₂ nanoparticles (Degussa P25) with respect to CF transformation kinetics and degree of CF mineralization. The tests are being conducted in UV projection-type batch reactors. Biogenic TiO₂ nanoparticles (Figure 1) were produced from marine diatoms as described by Rorrer's research group (Jeffryes et al., 2008). TiO₂ nanoparticles were often found as single particles. Thermal annealing at 680 °C converted the as-deposited TiO₂ to its anatase form with an average nanocrystal size of 19 nm, as verified by XRD, electron diffraction, and SEM/TEM.

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장소: 제주ICC

발표코드: ENVR1-4

발표분야: Abiotic/biotic Interactions in Nano-interfaces

발표종류: 심포지엄, 발표일시: 금 10:25, 좌장: 이우진

수계내 탄소나노튜브의 안정성에 대한 자연계유기물질의 영향

강석태, *C. D. Vecitis, **M. Elimelech

경희대 토목공학과 *Harvard University, USA **Yale University, USA

탄소나노튜브를 비롯한 다양한 나노물질은 화학적 안정성과 물리적인 강도, 전기특성등으로 인해 다양한 분야에 널리 응용되어왔다. 특히 탄소나노튜브는 환경공학분야에서 신개념 흡착제, 강도증가를 위한 첨가제 및 신개념 필터로 사용되었다. 반면, 나노물질의 응용범위가 확대됨에 따라 자연계로 배출되는 양 또한 잠재적으로 증가하였으며, 이로 인한 자연계 영향에 대한 사회적인 관심이 최근 고조되고 있다. 본 연구에서는 자연수계로 배출된 탄소나노튜브가 자연유기물질 (natural organic matter, NOM)과 상호작용할 때의 다양한 환경요인(pH, 이온강도)에 대한 영향을 평가하고 그 메커니즘을 규명하였다. NOM은 다양한 환경조건 변화 (pH 및 이온강도, 이온종류 변화)에 관계없이 탄소나노튜브에 효과적으로 부착하였으며, 부착한 NOM에 의해 탄소나노튜브의 안정도가 증가하였다. 탄소나노튜브 표면의 NOM 흡착량은 이온강도가 증가할 수록, Ca^{2+} 와 같은 2가 양이온이 존재할 수록 증가하였다. 메커니즘 규명을 위해 원자힘 현미경 탐침에 다중벽 탄소나노튜브 (multi-walled carbon nanotubes, MWNT)를 부착하고, MWNT-MWNT 사이에 존재하는 힘을 NOM 흡착 전후로 측정하였다. 실험결과, NOM이 존재할 때 수계내 탄소나노튜브의 안정도 증가는 부착된 NOM에 의해 발현되는 탄소나노튜브의 표면 음전하에 의한 정전기적 반발력때문이었으며, NOM의 흡착은 NOM내 aromatic ring과 탄소나노튜브 표면의 graphene 구조사이에 π - π 결합에 의한 것으로 밝혀졌다.

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장소: 제주ICC

발표코드: ENVR1-5

발표분야: Abiotic/biotic Interactions in Nano-interfaces

발표종류: 심포지엄, 발표일시: 금 10:50, 좌장: 이우진

Does nanoscale zero-valent iron affect iron-reducing/dechlorinating bacteria in the presence of trichloroethylene?

김영주, 박재우

한양대 건설환경공학과

Nanoscale zero-valent iron(nZVI) is increasingly used in environmental remediation of soil and groundwater due to its small size and high reactivity. However, little is known about the effect of nZVI on biological activity. In this study, we examined the interaction between nZVI and microorganisms, *Shewanella putrefaciens* and *Geobacter lovleyi*, on reductive dechlorination of trichloroethylene(TCE). Ferrous iron was reduced from nZVI shell, was increased in the *S. putrefaciens*-nZVI system. As a result of this iron reducing metabolism, the observed first-order degradation rate constants (k_{obs}) for TCE dechlorination increased from 0.0359 h^{-1} by only nZVI to 0.2324 h^{-1} by nZVI with *S. putrefaciens*. The experiment using *G. lovleyi*-nZVI system also exhibited the highest rate of TCE dechlorination. Hydrogen accumulation in nZVI was 1.2 mmol but in the reactors amended with *G. lovleyi* was accumulated only about 0.3 mmol after 168 h, indicating that most hydrogen produced was served as an electron donor. To investigate the differences between acetate or hydrogen as electron donor, we further studied the reduction of ferric iron in magnetite nanoparticles by *G. lovleyi* after aging nZVI. The addition of hydrogen slightly increased the iron reduction and acetate was not used as electron donor in the presence of hydrogen.

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장소: 제주ICC

발표코드: ENVR1-6

발표분야: Abiotic/biotic Interactions in Nano-interfaces

발표종류: 심포지엄, 발표일시: 금 11:15, 좌장: 이우진

Iron and Sulfur Biogeochemistry in Subsurface System: Coupled Biological and Geochemical Processes

권만재, 박영태, *윤현식, *이우람, *지민규, *지은도, 최재영

KIST 환경정화연구실 *연세대 환경공학과

Dissimilatory iron- and sulfate-reducing *Bacteria* (DIRB and DSRB) are common subsurface microorganisms as iron and sulfate are abundant in many natural environments. DIRB and DSRB couple the oxidation of organic carbon or H₂ to the reduction of iron and sulfate, which plays important roles in cycling of carbon, metals, and sulfur in the subsurface environment. DIRB and DSRB have also profound implications for the fate and transport of organic and inorganic contaminants in aquatic and terrestrial systems. Subsurface contamination by heavy metals or organic contaminants is a big concern for human health and environmental protection. In situ bioremediation is one option for reducing levels of contaminants. Introducing suitable substrates into the subsurface can stimulate the growth of iron and/or sulfate reducing microorganisms which often reduce contaminants either directly or by the production of reactive Fe(II) and sulfur species. In this presentation, we will discuss 1) the effects of several electron donors (i.e., acetate, lactate, and glucose) on the enrichment of specific communities capable of reducing iron and sulfate and 2) the effects of sulfate reduction on Fe^{III} (hydr)oxide (i.e., ferrihydrite, lepidocrocite, and goethite) reduction and microbial community development.

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장소: 제주ICC

발표코드: **ENVR1-7**

발표분야: Abiotic/biotic Interactions in Nano-interfaces

발표종류: 심포지엄, 발표일시: 금 11:40, 좌장: 이우진

Biomining of Nanomaterials and Their Application

노열

전남대 지구환경과학부

The objectives of this presentation are to show methods for producing nanomaterials by biological processes and to introduce their applications. A microbial process that exploits the ability of metal-reducing bacteria to produce copious amounts of extracellular nanomaterials has been developed. The metal-reducing bacteria isolated or enriched from diverse environments have ability to use short chain fatty acids as electron donors while reducing Fe(III), Cr(VI), U(VI), Co(III), and other redox sensitive metals at low temperature (2). The metal-reducing bacteria formed metal-substituted magnetites using iron oxide plus metals under conditions of relatively low temperature (< 70°C), ambient pressure, and pH values near neutral to slightly basic (pH = 6.5 to 9). The incorporation of transition metals into magnetite with the inverse spinel structure is of interest because of the unique magnetic, physical, catalytic, and electrical properties of such crystals. The bacteria also exhibited capabilities of formation of carbonate minerals such as siderite and rhodochrosite. These results indicate that microbial metal reduction and biomining of nanomaterials may play important roles in metal and carbon biogeochemistry as well as immobilization of metal contaminants in natural environments. The biological process rapidly produces copious amounts of nm-sized metal-substituted magnetite particles, which may expand the possible roles and utilities of nm-sized magnetic minerals.

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장소: 제주ICC

발표코드: **ENVR2-1**

발표분야: International Symposium on Future Energy Chemistry

발표종류: 심포지엄, 발표일시: 금 13:30, 좌장: 김태현

Electrolyte membranes using nano capping and pore-filling technologies for next generation PEFCs

Takeo Yamaguchi

Tokyo Institute of Technology, Japan

Protons rapidly conduct through unfreezable water in a micro pores, although many ions usually conduct through free water contained in polymer electrolytes. Pore-filling electrolyte membrane is a unique membrane that can suppress the swelling of filled polymer electrolyte because of its rigid porous substrate. Protons rapidly conduct through this structure. In addition, the activation energy of the proton conduction decreased from 16.3 to 9.1 kJ/mol in proportion to the increase in the ion exchange capacity (IEC) of the filled polymer, unlike the almost constant values of the usual-cast membranes. Also, we found that nano-particle inorganic electrolyte capped with polymer electrolyte showed high proton conduction through the interface between the two electrolytes under extremely low humidity condition. Coordination with pore-filling technology and nano-capping technology, durable and high performance electrolyte membranes are obtained. The membranes showed fast proton conduction at low to high temperature and low to high humidity conditions.

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장소: 제주ICC

발표코드: ENVR2-2

발표분야: International Symposium on Future Energy Chemistry

발표종류: 심포지엄, 발표일시: 금 14:00, 좌장: 김태현

Membrane Electrode Assembly for High temperature Polymer Electrolyte Fuel Cells

김형준

KIST 연료전지센터

Fuel cells offer several advantages for solving problems such as environmental contamination and fossil fuel diminishment. Among various kinds of fuel cells, polymer electrolyte fuel cells (PEFCs) have been in the spotlight because of their fast start-up, low operation temperature and high efficiency. However, low-temperature PEFCs (LTPEFCs) should be operated below 100 oC and water management has to be carefully controlled to achieve high performance of this type of cell. In addition, LTPEFCs demand CO (carbon monoxide)-free hydrogen as a fuel. For these reasons, high temperature PEFCs (HTPEFCs) (operating at >120 oC) have been studied to overcome the drawbacks of LTPEFCs. Most HTPEFCs employ acid-doped polybenzimidazole (PBI) derivatives in the fabrication of a fuel cell membrane. Although PBI itself does not have proton conductivity, it develops proton conductivity after being doped with a strong inorganic acid, such as phosphoric acid. Acid-doped PBI can be prepared by two different methods: post acid-doping with PBI membrane and in situ acid-doping by direct membrane casting from a polymerization mixture in polyphosphoric acid (PPA). The former method produces a membrane which has strong mechanical properties, but a limited doping level. The latter results in a high doping level, but low mechanical properties. In order to obtain an acid-doped PBI membrane for effective HTPMFEC operation, the two methods are used by carefully controlling the acid-doping level; however, there has been no solid strategy for fabricating a PBI membrane which has a high doping level, uses an easy membrane-casting method and exhibits strong mechanical strength. In this report, new membrane fabrication method is presented. Also, novel membrane electrode assembly (MEA) is reported. The MEA consists of 8 layers (1 phosphoric acid-doped PBI membrane, 2 electrodes, 1 sub-gasket, 2 gas diffusion media, 2 gas sealing gaskets). The sub-gasket mitigates the destruction of a highly acid-doped PBI membrane and provides long-term durability to the fuel cell stack.

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장소: 제주ICC

발표코드: ENVR2-3

발표분야: International Symposium on Future Energy Chemistry

발표종류: 심포지엄, 발표일시: 금 14:30, 좌장: 김태현

Synthesis and Properties of Sulfonated Aromatic Block Copolymers as Alternative Fuel Cell Membranes

Kenji Miyatake

University of Yamanashi, Japan

A series of sulfonated poly(arylene ether) block copolymers containing highly localized sulfonic acid groups have been synthesized for high temperature and low humidity operable fuel cells. Morphological observation revealed that high local concentration of sulfonic acid groups within the hydrophilic blocks enhanced hydrophobic/hydrophilic phase separation. The block copolymer membrane showed high proton conductivity comparable to that of the state-of-the-art perfluorinated ionomer (Nafion) membrane. The block copolymer membrane was hydrolytically stable in boiling water for 1000 h. Very low hydrogen and oxygen permeability was also confirmed. A fuel cell was successfully operated at 100 °C and 30% RH.

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발표코드: ENVR2-4

발표분야: International Symposium on Future Energy Chemistry

발표종류: 심포지엄, 발표일시: 금 15:10, 좌장: 임용범

Crosslinkable Poly(arylene ether) Membrane for PEMFC

이재석

광주과학기술원 신소재공학과, PIMS

Polymer electrolyte fuel cells have attracted a great deal of interest because of their potential applications as the alternative clean energy source in wide various applications. Currently, the most common perfluorinated sulfonic acid (PFSA) ionomers such as Nafion, which have excellent proton conductivity, good mechanical and chemical properties, and long-term durability, are commercially used. However, these ionomers not only limit the fuel cell operating temperature because of the low glass transition temperature, which leads to decrease mechanical property, but also have high fuel crossover. These problems of PFSA ionomers have stimulated many efforts in the development of alternative hydrocarbon based polymer electrolyte membranes. In this laboratory, polymer electrolyte membranes (PEM) based on thermal crosslinkable fluorinated-sulfonated poly(arylene ether) copolymers were prepared for fuel cell application. Introducing crosslinking system is a promising method among many kinds of sulfonated poly(arylene ether) copolymers, because it improves the membrane properties for instance decreasing water uptake and methanol permeability or increasing mechanical strength and thermal stability. The crosslinkable moiety of the copolymers was introduced into the end-group of polymer and/or the polymer main chain containing perfluorocyclobutyl(PFCB) or ethynyl group.

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발표분야: International Symposium on Future Energy Chemistry

발표종류: 심포지엄, 발표일시: 금 15:40, 좌장: 임용범

Facile Preparation of Photoanodes Thin Film with Photoelectrochemical Properties and Their Application

강영수

서강대 화학과

Ever since the French scientist Edmond Becquerel discovered the photoelectric effect, researchers and engineers have tried to get the photoelectrical system with the idea of converting light to electric power or chemical fuels. Their common dream is to capture the energy that is freely available from sunlight and turn it into the valuable and strategically important asset that is electric power, or use it to generate fuels such as hydrogen.¹ We demonstrated photoelectrochemical cells. One is that chemical fuel was produced by designed and controlled metal oxide photocatalysts. Their atomic structure and electronic structure was studied by Uv-vis, TEM, Raman, etc. The others are that photoelectrode was prepared with TiO₂, ZnO, CuO and NaTiO₂ for dye sensitized solar cells. Their morphology was controlled for photoelectrical properties and was characterized for application of dye sensitized solar cell. Keywords: Fe₂O₃, TiO₂, ZnO, CuO, Photoelectrode Reference 1. M. Grätzel Nature, 2001, 414, 338.

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발표분야: International Symposium on Future Energy Chemistry

발표종류: 심포지엄, 발표일시: 금 16:10, 좌장: 임용범

Artificial Photosynthesis: Coupling Biocatalytic and Photocatalytic Cycles for the Production of Valuable Compounds

류정기, 박찬범

KAIST 신소재공학과

Photosynthesis is a complex process in which plants produce essential biological fuels such as NAD(P)H and sugars from CO₂ and H₂O through solar energy. According to the photosynthetic Z-scheme, incident light electronically excites membrane-bound protein-pigment complexes called photosystem. The photogenerated electrons are rapidly delivered to reaction centers along the electron transport chain for regenerating NAD(P)H cofactors. These cofactors drive redox enzymatic reactions to synthesize organic compounds in the Calvin cycle. Inspired by the mechanism of natural photosynthesis, we have been developing artificial photosynthetic system which allows synthesis of valuable chemicals such as chiral compounds and drug intermediates by integral coupling of biocatalytic and photocatalytic cycles. We recently found that enzyme cofactors such as NAD(P)H can be successfully photoregenerated by using Rh-based organometallic compounds under visible light irradiation in the presence of light harvesting materials and used to drive enzymatic biocatalysis for the synthesis of valuable chemicals. Based on our findings, promises and challenges of artificial photosynthesis will be discussed in the symposium. References)1. C. B. Park, S. H. Lee, E. Subramanian, B. B. Kale, S. M. Lee, J.-O. Baeg, Chem. Commun. 2008, 5423-5425.2. S. H. Lee, D. H. Nam, C. B. Park*, Adv. Synth. Catal. 2009, 351, 2589-2594.3. D. H. Nam, S. H. Lee, C. B. Park*, Small 2010, 6, 922-926.4. J. Ryu, S. H. Lee, D. H. Nam, C. B. Park*, Adv. Mater., In Press (DOI: 10.1002/adma.201004576)5. S. H. Lee, J. Ryu, D. H. Nam, C. B. Park*, Chem. Commun., Accepted.

일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: **KCS1-1**

발표분야: Advances in Information Display Technology : Materials and Processing

발표종류: 심포지엄, 발표일시: 금 09:00, 좌장: 조길원

The Present and Future of Display Technology

박희동

한국화학연구원 디스플레이사업단

The flat panel displays (FPD) were replacing the CRT as the dominant devices for main stream applications. The most technology challenges in display are to produce higher performance devices with lower cost and also to find out new applications with an effective infrastructure, production technology, and new prototype devices. This presentation will feature a general trend and history of displays, a look at major FPD (LCD, PDP and OLED), world wide market of displays, and challenging issues on LCD, PDP and OLED for current displays and also on 3D, E-book and flexible display for future displays. In recent technology development, flexible display based on organic materials and printing methods represent one of the future displays, which are really bendable and designable displays like roll-up displays.

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발표코드: KCS1-2

발표분야: Advances in Information Display Technology : Materials and Processing

발표종류: 심포지엄, 발표일시: 금 09:30, 좌장: 조길원

Solution Processible Organic Semiconductors

권순기, *김윤희

경상대 나노신소재공학부 *경상대 화학과

Organic thin film transistors (OTFTs) have attracted much attention as alternatives with low-cost, large-area, and simple device structure to conventional silicon-based one. A number of p-type organic transistors have been reported so far, OTFT fabricated from a few materials show a comparable mobility to amorphous silicon based TFT. The most well-known OTFT materials is pentacene which has a mobility and on/off ratio of about 1 - 5 cm²/V.sec and 10⁷, respectively. However, Pentacene has several drawbacks such as, impossibility of solution process due to non-solubility in any organic solvent, and high cost etc. Especially, pentacene is very susceptible to some degradation in ambient conditions, presumably to form the endoperoxide or Diels-Alder adducts. Therefore, much more attention has been focused on designing new organic semiconductor candidates with high stability. In this presentation, we report the syntheses and characterization of new p-type OTFT materials. First, low molecular weight OSCs(Organic Semiconductors) of symmetric anthracene derivatives and asymmetric anthracene derivatives show high hole mobility and on/off current ratio by spin-coating method. Moreover, device exhibit high stability in the air condition. Second, polymeric OSCs of side chain conjugated polythiophene derivatives and naphthalene containing polymer show high mobility of 0.5 cm²/Vs and on/off current ratio by spin-coating method.

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발표코드: **KCS1-3**

발표분야: Advances in Information Display Technology : Materials and Processing

발표종류: 심포지엄, 발표일시: 금 10:00, 좌장: 조길원

Electronegative π -Conjugated Heteroaromatic Compounds as n-Channel OFET Materials

Yoshio Aso

Osaka University, Japan

It has been recognized that the introduction of electron-withdrawing groups into π -conjugated systems increases their n-type semiconducting character. We have designed and synthesized strongly electronegative heteroaromatic units, such as difluorodioxacyclopentathiophene, bis(dicyanomethylene)difluorocyclopentathiophene, and carbonyl-bridged bithiazole, and their based π -conjugated oligomers. Solubilizing units were further introduced to the oligomers for solution-processing applications. Some of their spin-coated thin films revealed high field-effect electron mobilities as well as air-stable n-channel FET operations.

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발표코드: **KCS1-4**

발표분야: Advances in Information Display Technology : Materials and Processing

발표종류: 심포지엄, 발표일시: 금 10:30, 좌장: 송정근

Solvent-free printing of organic semiconductors for high-performance organic electronics with a good scalability

유승협

KAIST

We present our study on a novel organic vapor-jet printing (OVJP) system in which deposition of organic materials is controlled point by point in a digital manner. It not only enables solvent-free deposition, mask-less pattern formation, and a good scalability, but also allows for use of well-established, sublime-grade small molecules that can promises both performance and long-term reliability. The overall concept of the proposed OVJP system and its operation are outlined, and the results of case studies utilizing the enhanced capabilities of the proposed OVJP methods are presented. An example includes high-performance organic thin-film transistors (OTFTs) based on organic materials printed by the proposed OVJP method. Finally, their potential applications are discussed from the perspectives of OLED displays as well other emerging devices.

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발표코드: KCS1-5

발표분야: Advances in Information Display Technology : Materials and Processing

발표종류: 심포지엄, 발표일시: 금 11:00, 좌장: 송정근

Semiconducting Polymer Electrospun Nanofibers

Chi-Ching Kuo, Cheng-Ting Wang, Jung-Yao Chen, *Wen-Chang Chen

*Institute of Polymer Science and Engineering *Institute of Polymer Science and Engineering and
Department of Chemical Engineering, National Taiwan University, Taiwan*

Electrospinning (ES) has emerged as a new technique to produce various functional nanofibers due to its advantages of low cost, high surface to volume ratio, and flexible morphology tuning. We are interested in exploring the morphology and optoelectronic properties of semiconductor polymer ES nanofibers, as described in the following: (1) Full color light-emitting ES nanofibers could be produced from the binary blends of polyfluorene (PFO) derivatives/PMMA. The PFO aggregation in the ES fibers was much smaller than that in the spin-coated film due to the ES geometrical confinement and resulted in higher luminescence efficiency. In addition, highly aligned ES nanofibers prepared from the ternary blends of PFO/poly(2,3-dibutoxy-1,4-phenylene vinylene)/PMMA led to the varied emission colors at different angles. (2) Novel electrospun (ES) fibers prepared from random copolymers of poly((2-(dimethylamino)ethyl methacrylate)-co-(stearyl acrylate)-co-(9,9-dihexyl-2-(4-vinylphenyl)-9H-fluorene)) exhibited the multi-functionality of thermo-responsive, physical crosslinking, and high fluorescence characteristics. (3) We have produced ES nanofiber field effect transistors (high hole mobility $> 0.3 \text{ cm}^2 \text{ V}^{-1} \text{ s}^{-1}$, On/Off $> 10^5$) from of regioregular polythiophene (P3HT) and two-dimensional conjugated polythiophene (P4DPP). The present study demonstrated that the above ES fibers prepared from semiconducting polymer systems could have potential application for sensory devices, smart textiles, optoelectronic, or nanoelectronic devices.

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발표코드: KCS1-6

발표분야: Advances in Information Display Technology : Materials and Processing

발표종류: 심포지엄, 발표일시: 금 11:30, 좌장: 송정근

The Development of Organic TFT Technology with Conventional Sputtered Metal Electrodes

김정한

LG디스플레이 Advanced TFT팀

The flexible display has been considered as one of the next generation displays to replace current displays such as LCD and PDP. Since the Organic TFT technology has promising characteristics including mechanical flexibility and low temperature processing that are available for flexible display fabrications, many researchers and companies have focused on the development of the Organic TFT technology. Although noticeable improvements have been achieved in the field of Organic TFT technology, two processing issues remain unsolved for the successful launching of the Organic TFT technology. One of the remaining issues is to replace high-priced gold metal with other cheap materials for source/drain electrodes. The other is metal sputtering process on the organic materials without any physical and electrical damage on it. In this presentation, the solutions for the above mentioned technical issues will be presented. Copper will be presented for source/drain materials and the surface treatment of the copper electrodes with SAM (Self Aligned Monolayer) will be introduced. TFT performance has been dramatically improved by SAM treatment and the performance with the copper source/drain after surface treatment shows very similar TFT characteristics to that with the gold source/drain. The metal sputtering process condition has been modified very carefully to minimize the damage of organic gate insulator and that condition will be represented. A modification of organic gate insulator material is also one of the critical factors to minimize plasma damage by conventional sputtering process. Finally, the EPD panel fully integrated with an organic TFT backplane will be introduced as well.

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장소: 제주ICC

발표코드: KCS1-7

발표분야: Advances in Information Display Technology : Materials and Processing

발표종류: 심포지엄, 발표일시: 금 14:00, 좌장: 권순기

Printed/Coated Non-volatile Displays with Electrochromic Nanoparticle Ink

Tohru Kawamoto, Hisashi Tanaka, *Masato Kurihara, *Masatomi Sakamoto

*AIST, Japan *Yamagata University, Japan*

Electrochromic displays (ECDs), a reflective one by means of a color change induced by electrochemical reactions, has been attracting keen interest because of its potential application as strong candidate for low-cost, high-volume electronic papers. One of the advantages of the ECDs is the high reflectivity of its white state. We developed the synthesis method of the electrochromic nanoparticles of Prussian blue $\text{Fe}[\text{Fe}(\text{CN})_6]_x$ and its metal-substituted analogues. With the nanoparticle, we can control the dispersibility by the surface modification. We synthesized the nanoparticles dispersible into water, alcohols, and organic solvents, indicating that we can fabricate the ECDs with the nanoparticles by coating or printing. Another advantages of the nanoparticle is enhancement of stability in electrochemical reactions. For example, we have succeeded in synthesizing $\text{Zn}[\text{Fe}(\text{CN})_6]$ nanoparticles showing stable electrochemical reactions by reducing its particle size less than 100 nm. Our ECD with Prussian blue nanoparticles exhibits color change between blue and white only with a 1.5 V dry battery even after operations of 1,000,000 times. The reflectivity of the white state is more than 50 %.

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장소: 제주ICC

발표코드: KCS1-8

발표분야: Advances in Information Display Technology : Materials and Processing

발표종류: 심포지엄, 발표일시: 금 14:30, 좌장: 권순기

Flexible OTFT-backplane using Printing Technologies

송정근

동아대 전자공학과

Flexible display is attracting much attention as an advanced display. Printing processes are essential technology for the flexible display considering their ability for large area deposition of thin films and the inherent low temperature process for plastic substrates and also low cost. In this paper we present the printing technologies for flexible OTFT-backplane. The various printing technologies were applied for each layers of OTFT; screen printing combining with reverse offset for gate electrodes and scan bus lines with Ag ink, spin coating for gate dielectric layer with PVP, ink jet for source/drain electrodes with PEDOT:PSS, ink jet for the semiconductor layer with TIPS-pentacene, and screen printing for pixels electrodes with Ag paste. The gate line width of 30 μm was reproducibly achieved with screen printing. Especially the resistivity of 10^{-6} ohm-cm was a meaningful result with screen printing. For S/D electrode conductivity of PEDOT:PSS was enhanced by doping with glycerol and was improved to 500 S/cm, which was sufficient enough for S/D electrodes. PEDOT S/D electrodes were patterned by ink jet and the channel length of 10 μm was obtained. The contact resistance with pentacene was comparable to that of Au. The dynamics of particle movement in a droplet was analyzed and applied to develop the process conditions to obtain the uniform layer of TIPS-pentacene. We could obtain the mobility of $0.3 \text{ cm}^2/\text{V}\cdot\text{sec}$ with deviation less than 10 %. An interlayer consisting of PVA and Acryl was coated on TIPS-pentacene. The final OTFT-backplane was obtained by screen printing the pixel electrodes with Ag paste. Finally 6 inch size of EPD sheet was laminated on the backplane. The EPD panel successfully demonstrated to display pictures.

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장소: 제주ICC

발표코드: KCS1-9

발표분야: Advances in Information Display Technology : Materials and Processing

발표종류: 심포지엄, 발표일시: 금 15:00, 좌장: 권순기

High performance inkjet-printed polymer based CMOS integrated circuits for a backplane of flexible displays

노용영

한밭대

Solution processed conjugated molecules enable to manufacture low cost various electronic devices by unconventional patterning methods such as inkjet, screen, or gravure printing with high throughput. Although the organic field-effect transistors (OFETs) using conjugated molecules as an active layer are not suitable for electronics requiring high charge carrier mobility due to intrinsic limitation of those materials, the advantage in manufacturing processes make them ideal for large-area, flexible, transparent, and disposable electronic devices such as drivers for flexible or transparent displays, digital circuits for radio frequency identification (RFID) tags, sensors, and memories. Moreover, the charge carrier mobility of state-of-the-art organic semiconductors is comparable with amorphous silicon so that it is expected that many applications will be replaced by cost-effective solution processed OFETs in near future. To realize advanced integrated CMOS circuits, those p-channel or n-channel conjugated molecules must be patterned. However, conventional patterning process such as photolithography is not suitable since conjugated molecules are very weak under UV light illumination and cost of manufacturing facility is also very high. Therefore novel patterning methods have researched so far such as micro contact printing, inkjet printing. Among those novel patterning methods, inkjet has a variety of advantages such as removal of need for masks, which lead to cost-savings, efficient use of materials and waste elimination, non-contact deposition method (little contamination). Here we demonstrate high performance inkjet printed p-channel and n-channel top-gate/bottom-contact polymer field-effect transistors (FETs), and applications to elementary organic complementary inverter and ring oscillator circuits. We have obtained high field-effect mobility more than $0.3 \text{ cm}^2/\text{Vs}$ for both of p-channel and n-channel FETs, and the CMOS polymer ring oscillator showed very high operating frequency of 50 KHz. In addition, we achieve

the high resolution inkjet printing method for gate line printing for top gated OFETs and integrated circuits.



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발표코드: **KCS1-10**

발표분야: Advances in Information Display Technology : Materials and Processing

발표종류: 심포지엄, 발표일시: 금 15:30, 좌장: 노용영

Low-temperature Solution-processed TFT for Display Applications

김보성

삼성전자 LCD 연구소

The increasing demand for solution-processed TFTs has given an boost to the development of soluble organic and metal oxide semiconductors. They could be core materials to realize low-cost, flexible and roll-to-roll process for the applications of LCD, OLED as well as new future displays. Organic semiconductors has been studied mainly focused on the improvement of their electrical stability, being considered a TFT backplane of e-paper display. On the other hand, the solution type of metal oxide semiconductors has been paid a lot of attention because of their high charge carrier mobility, high optical transparency, excellent chemical stability, and processing versatility. In this talk, Samsung's recent progress of solution-processed TFTs will be presented including the fabrication of TFTs with soluble organic semiconductors and oxide semiconductors, and their electrical characteristics respectively for display applications.

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발표코드: **KCS1-11**

발표분야: Advances in Information Display Technology : Materials and Processing

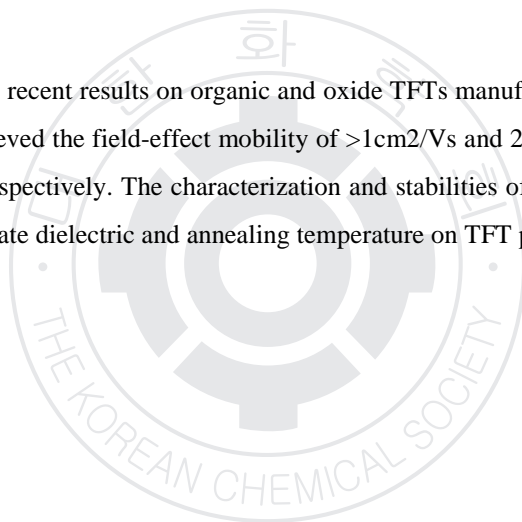
발표종류: 심포지엄, 발표일시: 금 16:00, 좌장: 노용영

Solution processed TFTs for large-area electronics

장진

ADRC & Department of Information Display, Kyung Hee University

In this talk I will review the recent results on organic and oxide TFTs manufactured by using spin casting and inkjet printing. We achieved the field-effect mobility of $>1\text{cm}^2/\text{Vs}$ and $20\text{cm}^2/\text{Vs}$ for TIPS pentacene and zinc-tin-oxide TFTs, respectively. The characterization and stabilities of the TFTs will be presented, together with the effect of gate dielectric and annealing temperature on TFT performance.



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발표코드: KCS1-12

발표분야: Advances in Information Display Technology : Materials and Processing

발표종류: 심포지엄, 발표일시: 금 16:30, 좌장: 노용영

Organic Transistors Based on Conjugated Molecules / Polymer Blends

조길원

포항공과대 화학공학과

Organic semiconductor and insulating polymer blends have been attracting considerable attention for organic thin-film transistors (OTFTs) because the electronic properties of organic semiconductors can be combined with the low-cost and excellent mechanical characteristics of insulating polymers. Here, we demonstrate that excellent electrical properties of OTFTs based on blend films can be obtained by fabricating two unique structures, vertically phase-separated structure and interconnected semiconducting nanowires embedded in insulating polymer. Firstly, semiconductor-top and insulator-bottom bilayer structure was fabricated by surface-induced vertical phase separation of poly(3-hexylthiophene) (P3HT) and poly(methyl methacrylate) blends. This bilayer structure exhibits the improved TFT characteristics even at content of P3HT as low as 5%, as well as one-step fabrication of low-voltage-driven device. Further, we demonstrate that the controlled solubility using marginal solvent or solvent mixture in blends of P3HT and amorphous polystyrene (a-PS) allows blend film to have the unique structure with P3HT nanowires embedded in PS matrix. The P3HT molecules in these blends form highly crystalline, interconnected nanowire networks dispersed in PS matrix, which is extremely beneficial for keeping connectivity at content of P3HT as low as 1 wt% and improving environmental stability. In addition, the embedded nanowire network structure can be successfully produced by using inkjet printing technique for the direct-write fabrication of TFTs.

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장소: 제주ICC

발표코드: KCS2-1

발표분야: 2011 East Asian Symposium on Molecular Electronics Materials

발표종류: 심포지엄, 발표일시: 금 09:10, 좌장: 김은경

Supramolecular control of ultrafast photoresponses for molecular photonics

Toshihiko Nagamura, Yasuhiro Sota, Tomonori Ono, Kaoru Kawasaki, Keiji Tanaka

Kyushu University

Molecular and polymer materials are essential in advanced information society. We have been developing various materials and devices for ultrafast all-optical processing and switching based on single electron transfer in the visible to optical telecommunication wavelength region. We have demonstrated 4,4'-bipyridinium derivatives containing electronic conjugation systems with various length between two pyridinium units work as acceptors showing photoinduced electrochromism in a broad wavelength region. The ON response due to photoinduced electron transfer occurs in less than 0.1 picoseconds (ps) upon excitation of ion-pair charge transfer complexes. But the time constants of OFF response are not uniform ranging from 0.24 ps to a few hundred ps due to distribution of distance and/or orientation between oxidized donors and reduced acceptors. We have also proposed a composite polymer guided wave mode geometry to control signal light very sensitively by gate light in a parallel way through photoinduced complex refractive index changes of molecules or polymers. Very recently we also succeeded to make reverse reactions a single exponential by employing various 4,4'-bipyridinium derivatives with a linked neutral aromatic donor and nanocavity molecules to entrap them. By this way we have achieved ultrafast OFF responses without slow components in the visible to optical telecommunication wavelength region. It is most probably attributed to intramolecular charge transfer complex formation in confined nanocavities to make uniform conformation between donors and acceptors. The present result will contribute a great deal to make future ultrafast all-photonic networks based on organic molecules and polymers.

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장소: 제주ICC

발표코드: **KCS2-2**

발표분야: 2011 East Asian Symposium on Molecular Electronics Materials

발표종류: 심포지엄, 발표일시: 금 09:35, 좌장: 김은경

Our Recent Progress on New Materials to Harvest Light

Pi-Tai Chou

Nat'l Taiwan University

This talk will cover a topic that is currently studied in my lab, namely strategic design and synthesis of new materials suited for DSSCs and OPV. Several prototypes will be demonstrated to underline their associated fundamentals and latent applications. Of particular interest are derivatives of ortho-GFP core molecule that undergo proton transfer in the excited state.^{1,2} Recent advances on the progress of Ru(II) complexes in DSSCs will be presented as well.³ The device configurations are also focused in an aim to optimize the cell performance and to extend future versatility. If there is some time left, the topic will cover development of certain nanocomposites and their applications toward photovoltaic applications. One focus should be hybrid solar cell containing semiconducting nanomaterials and D-A -conjugated lower band-gap polymer.

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장소: 제주ICC

발표코드: KCS2-3

발표분야: 2011 East Asian Symposium on Molecular Electronics Materials

발표종류: 심포지엄, 발표일시: 금 10:00, 좌장: 김은경

An Effective Tool for Micro Devices- Two Photon 3D Stereolithography

이광섭

한남대 신소재공학과

One of the important nonlinear optical properties is two-photon absorption (TPA) in which some molecules can absorb simultaneously two photons, when irradiated by intense laser pulses. The rate of TPA scales quadratically whereas the rate of one-photon absorption linearly increase with the intensity of the incident radiation. The rate also depends upon the TPA cross-section of the molecule. TPA materials with a large cross-section can be utilized for photonic and bio applications such as for two-photon-excited fluorescence microscopy, optical power limiting, three-dimensional optical data storage, photodynamic therapy and two-photon induced biological caging studies as well as stereolithography by two-photon initiated polymerization (TPP). Here, considerable efforts focusing on TPP have been put forth in the area of two- and three-dimensional (2D and 3D) nano/ microfabrication for the development of new conceptive nano/micro-devices. Since TPP first came out as a novel technique over a decade ago, a great number of diverse micro-objects have been fabricated using TPP with a variety of effective two-photon chromophores. In TPP, when a near-infrared ultrashort-pulsed laser is closely focused into a volume of photocurable resins, real 3D microstructures can be fabricated using a layer-by-layer accumulating technique; therefore, TPP is considered to be a promising technique for 3D nano/ microfabrication. Recent reports have shown that the spatial resolution of TPP is achieved at approximately the sub-100 nm scale over diffraction limit of incident light. However, a few studies have been carried out especially based on improving the fabrication efficiency and precision of TPP. In this presentation, we report our attempts to improve the fabrication efficiency of nano/ microfabrications based on TPP.

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발표코드: KCS2-4

발표분야: 2011 East Asian Symposium on Molecular Electronics Materials

발표종류: 심포지엄, 발표일시: 금 10:25, 좌장: 김은경

Photocatalytic reactions on layered titanates: Designed nanostructures for controlled reactions

Makoto Ogawa

Waseda University

Titania base materials have been attracted much attention due to their useful properties including photocatalytic abilities. In order to optimize the useful properties, titania based materials have been synthesized to control the morphology (for example, nanoparticles, films) and the structures. Among possible titania based materials, layered titanates are materials with versatile applications including filler, ion exchanger and photocatalyst.¹⁻⁶ Possible surface modification of layered titanates with organic functionality by the reactions with silane coupling reagents make the materials more attractive.¹ We have already reported the functionalization of layered titanate by ion exchange² and grafting¹ for possible application as filler,³ adsorbent,⁴ and photocatalysts.⁵ In this talk, photocatalytic applications of layered titanates will be introduced to show the merits of nanostructure design. A layered titanate, $\text{K}_{0.66}\text{Ti}_{1.73}\text{Li}_{0.27}\text{O}_{3.93}$, was used for photooxidation of organic compounds in water and the efficiencies and the substrate selectivity was successfully modified by the ion exchange of the interlayer potassium ions.⁵ The immobilization of gold nanoparticles on TiO_2 particulates has attracted attentions to achieve visible light-induced photocatalysis such as the oxidation of aqueous organic substrates.⁷ Gold nanoparticles-loaded titania seems to be advantageous because of the size and morphology-dependent light absorption of gold nanoparticles from visible to near infrared region. Gold nanoparticles were deposited in the interlayer space of a layered titanate to give nanoporous material with molecular-sieving ability. The present hybrid catalyzed the direct oxidation of benzene to phenol by visible light irradiation. Immobilization of photosensitizing dyes on layered titanate is a way to prepare visible light responsive photocatalysts.^{8,9}

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발표코드: **KCS2-5**

발표분야: 2011 East Asian Symposium on Molecular Electronics Materials

발표종류: 심포지엄, 발표일시: 금 11:10, 좌장: Toshihiko Nagamura

Novel Luminescent Probes with Excited State Intramolecular Proton Transfer and Charge Transfer

Guoqiang Yang

Inst. Chem. Chin. Acad. Sci

Excited state intramolecular proton transfer (ESIPT) compounds and intramolecular charge transfer (ICT) compounds have attracted much attention for their luminescent properties. The luminescence of the compounds is sensitive to the environment. For the ESIPT compounds, a fast four-level photophysical cycle occurs immediately after photo-excitation. The emission from the proton transfer state gives abnormally large Stokes shift and no self-absorption is detected. For the ICT compounds, the emission shows red shift with increasing of the solvent polarity. Meanwhile, significant changes of the luminescent properties are observed from solution to aggregation. For the good stability and unique luminescent properties, ESIPT compounds and ICT compounds are expected to be potential intrinsic luminescent materials and some novel compounds are used as luminescent probes for the detection of ions, temperature and VOCs.

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발표코드: **KCS2-6**

발표분야: 2011 East Asian Symposium on Molecular Electronics Materials

발표종류: 심포지엄, 발표일시: 금 11:35, 좌장: Toshihiko Nagamura

Real-time Face-to-Face Communication by Photonic Polymers

Tetsuya Toma, Yasuhiro Koike

Keio University

Recent progress and status of photonic polymers for overwhelmingly realistic face-to-face communication are described. The world's fastest graded-index plastic optical fiber covering 40gbps which is directly connected to large size display realizes remote face-to-face communication with high realistic sensation without time lag. The 3D 4K display has been successfully made by a highly scattered optical transmission polymer which increases the brightness and contrast, and by an invention of zero-birefringence polymer which dramatically improves the control of polarization phase and dissolves the mura problem at low fabrication cost. The key technology is the photonic polymer which will totally change the communication system of today.

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발표코드: **KCS2-7**

발표분야: 2011 East Asian Symposium on Molecular Electronics Materials

발표종류: 심포지엄, 발표일시: 금 12:00, 좌장: Toshihiko Nagamura

Organic electronics from micro structured active polymer films

김은경, 김유나, 김정훈, 김병관, 유정목

연세대 화공생명공학과

The electrical and optical properties of active polymers are essential for the performance of organic electronics. Those properties could be controlled at the organic molecular level by optimizing chemical as well as domain structure of active polymers. While most of the efforts concerned on micro scale fabrication process for electronic devices, we have developed active polymer films that utilize functionalized monomers. The monomers were tailor-made to control band gap and microstructure of active polymer film. With a microscale pattern, the active polymer film showed enhanced optical and electrochemical properties. A photo cross-linkable and vapor phase polymerizable monomer afforded simple process for conductive micro circuit and thin film display. Emphasized here are monomers for the formation of active polymer channels in nanophase template, to give high functionality. This allowed a facile method for the preparation of organic electronics such as electrochemical displays with color tunability and an iodine-free ssDSSC with excellent energy conversion efficiency in a simple structure.

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발표코드: **KCS2-8**

발표분야: 2011 East Asian Symposium on Molecular Electronics Materials

발표종류: 심포지엄, 발표일시: 금 14:00, 좌장: 이광섭

Surface Plasmon Resonance Effect on Photofunctional Polymer Nanosheet Assemblies

Tokuji Miyashita, Masaya Mitsuishi

Tohoku University, Japan

We have developed photofunctional devices based on polymer nano-sheet assemblies. In the hybrid assemblies of polymer nanosheets with metal nanoparticles, the photofunction such as photo-electric conversion, photoluminescence and nonlinear optics is strongly enhanced by coupling with metal nanoparticles. This is caused by Surface Plasmon Resonance. In this presentation we will introduce interesting new topics and the mechanism working in the assemblies.

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발표코드: **KCS2-9**

발표분야: 2011 East Asian Symposium on Molecular Electronics Materials

발표종류: 심포지엄, 발표일시: 금 14:25, 좌장: 이광섭

Designing Torsion Spring Molecules for Molecular Electronics Application

박수영

서울대 재료공학부

In this presentation, I will introduce our recent works on designing nano-structured organic heterojunction which comprises interfacial layers of carrier accumulation or depletion. Specific properties of conductivity, photoconductivity, charge transfer, exciplex formation, and photovoltaic effect are correlated with the energy levels of the specific heterojunction which consists of p-type conjugated polymer and n-type torsion spring molecule. In the second part of this presentation, a unique pizochromic fluorescence will be demonstrated for the fluorescent organic crystal made of a special torsion spring molecule.

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발표분야: 2011 East Asian Symposium on Molecular Electronics Materials

발표종류: 심포지엄, 발표일시: 금 14:50, 좌장: 이광섭

Supramolecular Approach for Luminescent Organic Solids – Switching of Solid Luminescence

Koji Araki

University of Tokyo, Japan

Luminescent organic solids have been the subject of intense ongoing studies because of the potential for their use in photonic and photoelectronic devices, though there are various excited-energy dissipation processes in the solid state. Among them, supramolecular approach for tuning and switching of solid-state luminescence has been attracting considerable interest in recent years.¹ By controlling mode of the molecular packing by external stimuli, on-off or color switching of the luminescence has been realized. In order to attain this goal, stimuli-responsive molecular packing and effective mechanism for packing-to-luminescence transduction have to be designed and realized. In this presentation, use of multiple hydrogen bonds as the key intermolecular interaction is discussed as an effective design concept for fabrication of stimuli-responsive molecular packing.² Based on the recent results on polymorph-dependent excited-state intramolecular proton transfer (ESIPT) luminescence of 2-hydroxyphenylimidazo[1,2-a]pyridine (2-OHPIP) derivatives, the effective mechanism for the packing-to-luminescence transduction is also discussed in terms of their excited states and the mode of molecular packing.³

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발표분야: 2011 East Asian Symposium on Molecular Electronics Materials

발표종류: 심포지엄, 발표일시: 금 15:15, 좌장: 이광섭

Spin injection and transport in organic semiconductors

Hirokazu Tada

Osaka University

Considerable attention has recently been paid to the active control of spin degrees of freedom in organic materials (OMs), since the long spin diffusion length is expected to be exhibited in OMs composed of light elements. The understanding of spin-injection and transport characteristics in low molecular weight OMs is particularly of importance, since it is feasible to optimize molecular structures for improvement of device performance by chemical design as has been demonstrated in the research field of molecular electronics. There are, however, still some arguments whether spins are just tunneling between electrodes or are transported in organic materials. We have prepared layered and planar type sandwich structures of Co/organic/LSMO ($\text{La}_{0.7}\text{Sr}_{0.3}\text{MnO}_3$) and LSMO/organic/LSMO, respectively, with various materials such as Alq₃, C₆₀, pentacene, phthalocyanine, TPD (1,1'-bis(4-di-*p*-tolylamino-phenyl)cyclohexane) and BTQBT (bis (1,2,5-thiadiazolo)-*p*-quinobis (1,3-dithiole)), and measured spin-valve characteristics of the devices at various spacer length. It was found that the polarity of magnetoresistance (MR) in layered devices varied depending upon the materials as well as their thickness. All devices with thin organic layers showed inverse MR. While the devices with thick films of electron transporting materials such as Alq₃ and C₆₀ showed also inverse MR, those with thick TPD, phthalocyanine and pentacene (hole transporting materials) films showed normal MR. This indicates that molecular orbitals of organic materials play an important role in spin transport.

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발표분야: 2011 East Asian Symposium on Molecular Electronics Materials

발표종류: 심포지엄, 발표일시: 금 16:00, 좌장: Hirokazu Tada

Extraction of emitted light in organic light emitting diodes

김장주

서울대 재료공학부

As the internal quantum efficiency of organic light emitting diodes (OLEDs) approaches 100% by development of phosphorescent dyes and optimizing device structures, the external quantum efficiency is mostly determined by the outcoupling of emitted light in OLEDs. First part of this talk will discuss the theoretical estimation of the maximum outcoupling efficiency in conventional OLEDs using a classical electromagnetic theory. The analysis predicts that the maximum outcoupling efficiency can be 30% which is much higher than commonly believed 20%. Still rest of the emitted light is waveguided along the organic or ITO layers or trapped in glass substrate or absorbed by surface plasmon polaritons in metal electrodes. Extraction of the waveguided light is important to improve the efficiency of OLEDs for displays and solid state lighting. Second part of this talk will present a few methods to improve the outcoupling efficiency of single color OLEDs and white OLEDs, which include the nanostructures between transparent conducting oxides and glass. The results will be discussed based on optical calculation

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발표분야: 2011 East Asian Symposium on Molecular Electronics Materials

발표종류: 심포지엄, 발표일시: 금 16:25, 좌장: Hirokazu Tada

New functional dyes for organic solar cells

He Tian

East China Univ. of Sci. Tech., China

Triarylamine has been widely used in opto- and electro-active materials for its good electron donating and transporting capability, as well as its special propeller starburst molecular structure. Recently, organic photovoltaic functional materials with triarylamine as electron donor have aroused great interest and become the focus of intensive research in the field of solar cells. For metal free organic sensitizers based on triarylamine, the power conversion efficiency is enhanced by its nonplanar propeller molecular geometry, which prohibits the undesirable close molecular aggregation and the charge recombination. Moreover, the excellent stability of triarylamine contributes to the cell durability. Heterojunction solar cells based on triarylamine sensitizers show good performance due to the excellent electron donating and transporting capabilities as well as aggregation inhibition character of triarylamine. The introduction of triarylamine units has significantly facilitated the development of organic solar cells.

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발표분야: 2011 East Asian Symposium on Molecular Electronics Materials

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Aggregation-induced red emissive NPAFN showing high field-effect transistor mobility and very large open circuit voltage ~ 1 V in organic photovoltaics application

Chin-Ti Chen

Inst. Chem. Acad. Sinica, Taiwan

Efficient organic photovoltaic device (OPVs) have been realized by using an aggregation-induced emission (AIE) red fluorophore bis(4-(N-(1-naphthyl)phenylamino)phenyl)fumaronitrile (NPAFN) as electron donor in planar double heterojunction OPV containing C₆₀ as electron acceptor and bathocuproine as exciton blocking layer adjacent to Al cathode. NPAFN exhibits a high hole drift mobility greater than 0.07 cm²/Vs, determined by its field-effect transistors. Although it has a relatively short absorption wavelength ($\lambda_{\text{max}} < 500$ nm), NPAFN OPV shows high performance: open circuit voltage V_{OC} of 0.99 V, short circuit current J_{SC} of 3.7 mA/cm², fill factor FF of 62%, and power conversion efficiency η_{PC} of 2.25%. Having same device structure of OPV, such performances (V_{OC}, FF, and η_{PC}) are better than those long wavelength absorption ($\lambda_{\text{max}} > 600$ nm) electron donor pentacene, copper phthalocyanine, or boron subphthalocyanine chloride.

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발표분야: 2011 East Asian Symposium on Molecular Electronics Materials

발표종류: 심포지엄, 발표일시: 금 17:15, 좌장: Hirokazu Tada

The Characteristics of OTFT fabricated by Printing Blended Organic Semiconducting Inks

이창진

한국화학연구원 화학소재연구본부 소자재료연구팀

Printing organic thin film transistors and using them in the electronic circuitry are getting more attractive and wide spread technology. In addition to the merits of the less energy consuming process and less capital investment for the building the manufacturing factories, the capability of producing the light-weighted and thin-flexible electronics makes the printing electronics one of the most promising technology of the future electronic technology. Many organic semiconducting materials have been developed for the channel materials of the transistors and some of them showed good properties as the mobility exceeding the amorphous silicon. For example, the mobility of bis(triisopropylsilyl)ethynyl-pentacene (tips-pentacene) is reported to give higher than $1 \text{ cm}^2/\text{V}\cdot\text{s}$ and it is highly soluble in most organic solvents. The processibility of this small molecules could be modified by blending with some other binder polymers and the blended mixturse showed that they could be serve as an excellent inks. In our study, we also develop some new polymers containing triarylamine unit and used them as binder polymers. Depending on the molecular structures of the binders and processing conditions, we observed the mobilities in the range for 0.1 to $0.6 \text{ cm}^2/\text{V}\cdot\text{s}$ and improvement in long term stability of the printed transistors.

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발표분야: Chemistry for Conservation of Cultural Properties

발표종류: 심포지엄, 발표일시: 목 14:00, 좌장: 도진영

부여 능산리사지 유리제품의 성분조성과 계통에 관한 연구

강형태, *고민정, **김연미

국립중앙박물관 보존과학팀 *공주대 문화재보존과학과 **국립부여박물관 학예연구실(보존과학실)

부여 능산리사지 제 2 차 조사에서 공방관련 유구를 발견하였다. 이 공방지의 중앙실에서 금동대향로를 비롯한 각종 금동제품, 철부, 칠토기, 유리제품 등 가장 많은 유물이 출토되었다. 출토된 유리제품은 수백 점에 이르며 대부분 구슬로서 색상과 종류가 다양하다. 이 중 수습과정에서 독특한 유리가 발견되었는데 감청색의 깨진 잔편들과 연한 황갈색 바탕에 갈색 줄무늬가 들어 있는 유리이다. 이 유리 편에서는 구연부가 확인되어 유리용기에서 떨어져 나온 파편이라는 것을 알 수 있었다. 따라서 본 연구에서는 다양한 색상을 띠는 유리구슬 18 점(황색, 주황색, 벽색, 적색, 녹색, 투명한 황색, 은박유리)과 서역 유리용기로 추정되는 편 6 점(황갈색 줄무늬유리, 감청색)을 대상으로 비중, 조성분석, 주성분분석을 실시하여 각각의 유리에 대한 화학적 특성을 확인하였다. 또한 서역 용기편으로 추정되는 유리가 실제 서역 유리의 특성을 가지고 있는지, 그렇다면 로마 계인지, 사산 계인지 여부를 밝히는 과학적 근거를 제시하였다. 그리고 기 분석한 황남대총의 일부 유리용기 편과의 관계성 여부를 검토하였다. 이 결과 전체적인 유리편의 비중은 2.0~3.0 범위이며, 성분조성은 모두 소다유리계통으로 안정제의 함량에 따라 전형적인 아시아계통의 유리인 LCHA 그룹, 서역계통의 HCLA 그룹으로 나뉘었다. HCLA 그룹에서 3 점(황갈색 은박유리구슬 1, 구슬 1, 황갈색 줄무늬 유리용기 편 1)은 사산 계로, 감청색 유리용기 잔편은 로마 계인 것으로 판단된다. 그리고 능산리사지 은박유리구슬은 무령왕릉의 은박유리구슬과도 성분조성이 일치한다는 것을 확인하였고, 황색과 녹색 유리구슬의 착색제는 PbSnO_3 (lead tin oxide)라는 것 또한 알 수 있었다. 능산리사지 황갈색 줄무늬유리(번호 24)는 황남대총의 무색투명 유리와 사산 계로서 동일 그룹에 포함된다. 이러한 결과는 유리용기 제조를 위해 사용한 원료 및 배합비가 동일하다는 것을 의미한다.

감청색 유리용기는 능산리사지와 황남대총에서 모두 볼 수 있는데 원료 배합 비에 약간의 차이가 있어 서로 다른 제작지에서 만들어졌을 가능성이 높다. 이와 같은 연구는 한국 고대유리 문화를 과학적으로 해석하는데 있어서 중요한 기초자료로 활용될 수 있다.



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발표분야: Chemistry for Conservation of Cultural Properties

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한국에서 출토된 박 유리구슬의 고고화학적 연구

김나영, 김규호

공주대 문화재보존과학과

박 유리구슬은 내형 유리, 금속박, 외형 유리의 3 중 구조로 이루어진 환옥 혹은 연주옥으로 한국에서 출토된 고대유리 중에서 특이형으로 분류된다. 따라서 본 연구는 박 유리구슬의 유리와 금속박에 대한 미세구조 관찰과 주성분 및 미량성분 분석을 통해 제작 기법과 재질적 특성을 확인함으로써 당시의 기술 수준과 고대유리 문화의 변천 및 유통 경로를 이해하고자 하였다. 연구 대상은 2 세기부터 7 세기 이르는 연천 학곡리, 김해 양동리, 아산 탕정, 고창 남산리, 천안 두정동, 공주 무령왕릉, 나주 복암리 등 7 개 유적에서 34 점을 선정하였다. 박 유리구슬의 금속박은 금박과 은박으로 구분되며, 대부분은 금박유리이나 무령왕릉에서 처음으로 은박유리가 확인되었다. 유리는 내구성을 높이기 위해 CaO 가 사용된 소다유리로 소다를 얻기 위해 첨가한 원료가 광물과 해양 식물의 재로 구분된다. 광물 원료가 사용된 유리는 유리의 색상이 무색을 띠는 금박유리로 한국에서 출토된 박 유리구슬의 일반적인 형태인 반면 식물 재 원료가 사용된 유리는 유리의 색상이 황색과 무색을 띠는 금박 및 은박유리로 연천 학곡리와 무령왕릉에서 한정되어 확인된다. 이와 같은 조성은 당시 광물을 사용한 로마 유리와 해양 식물 재를 사용한 사사니안 유리와 유사성이 높으므로 유입 경로에 차이로 해석될 수 있을 것으로 기대된다. 미량성분에서 식물 재가 사용된 유리는 동일 그룹을 형성한 반면 광물 원료가 사용된 유리는 3 개 그룹으로 구분된다. 양동리, 탕정, 남산리, 두정동 그리고 일부 복암리 금박유리는 유적의 편년 및 지역 차이에도 불구하고 원료의 상관관계가 높게 나타났으나 연천 학곡리와 나주 복암리에서 출토된 금박유리 일부는 각각 그룹을 형성하여 사용 원료의 다양성이 확인된다.

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파주 혜음원지 출토 청자의 고고화학적 특성 연구

고민정, 김규호

공주대 문화재보존과학과

파주 혜음원지는 고려시대에 개경과 남경의 교통 요지에 건립된 일종의 국립숙박기관으로 이 유적에 대한 발굴조사결과 다량의 청자와 중국자기 일부가 출토되었다. 청자의 기종은 접시, 대접, 완, 바리때 등 일상용기가 대부분이며, 압출양각, 상감, 퇴화, 철화 등 다양한 기법이 사용되었다. 이러한 청자의 양상은 고려 중기 청자의 전반적인 특성을 제시한다는 측면에서 중요하다. 따라서 본 연구에서는 혜음원지 청자를 대상으로 색도, 흡수율 및 기공률, 태토의 주성분과 미량성분, 유약의 주성분, 미세구조 관찰을 실시하여 기종에 따른 혜음원지 청자의 물리·화학적 특성을 파악하였다. 또한 혜음원지 청자의 생산지로 추정되는 지역의 기 발표된 청자 데이터와 비교·검토하여 생산지에 대한 과학적 근거를 제시하고자 하였다. 분석결과를 살펴보면 혜음원지 청자태토의 색상(L^* , a^* , b^*)은 (65.1, 0.4, 1.7), 유약(L^* , a^* , b^*)은 (55.0, -5.2, 6.7)과 (53.7, -2.3, 9.3)의 값을 갖는다. 비중 및 흡수율, 기공률은 치밀한 시편의 경우 2.20, 1.2 %, 2.2 %, 치밀도가 낮은 시편의 경우 2.16, 2.3 %, 4.2 %로 측정되었다. 미세구조는 시편의 자화도에 따라 차이가 나타나고 있으며, 이는 앞서 서술한 비중 및 흡수율과 연관성이 있는 것으로 확인된다. 주성분 분석 결과 태토는 실리카 72~77 %, 알루미나 16~19 %, 2 % 내외의 철산화물, 5 % 이하의 용제성분을 함유하고 있다. 유약은 실리카 58~64 %, 알루미나 13~15 %, 2 % 이내의 철산화물, 0.3 % 정도의 산화티타늄이 착색제로 작용하고 있다. 인산화물은 0.5 % 이하이며 용제 성분의 총합은 25 %이다. 혜음원지 청자 시편에 대한 주성분 분석에서 태토와 유약의 조성은 기종별로 분류되지 않으며, 기 발표된 유적(강진 용운리-사당리-삼흥리-계율리, 해남 진산리-신덕리-조송리, 부안 진서리-유천리, 고창 용계리) 출토 청자와 미량성분 함량을 비교한 결과에서 강진 사당리, 부안 유천리-진서리 청자와 상대적으로 높은 유사성이 확인된다.

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장소: 제주ICC

발표코드: KCS3-4

발표분야: Chemistry for Conservation of Cultural Properties

발표종류: 심포지엄, 발표일시: 목 15:00, 좌장: 도진영

관요 설치 이후 조선 백자의 화학성분과 제작기술 특성

이영은

경기도박물관 보존과학실

경기도 광주에 설치된 관요(官窯)는 조선시대 왕실에서 사용하는 도자기를 국가가 직접 담당하여 제작하는 관영자기제조장이다. 1466-1469년 경 관요 설치 이후, 도자기의 체계적인 생산시스템이 구축되고 원료가 안정적으로 공급되면서 제작기술 측면에 있어서도 비약적인 발달이 이루어졌다. 15세기 후반과 16세기 전반에 제작된 회고 치밀한 태토와 매끈하고 은은한 유색을 지닌 백자는 18세기 청화백자와 더불어 조선백자의 최고 수작(秀作)으로 꼽힌다. 또한 이 시기에는 사용처에 따라 굵의 형태와 굵받침, 갑발의 사용여부 등 자기의 형태와 번법에 차이를 두어 제작하는 이원화된 제작구조를 보인다. 본 연구에서는 이러한 생산체계의 변화에 따른 백자의 기술적인 특성을 다양한 과학적 분석을 통하여 규명하고자 하였다. 분석에는 XRF-WDS, SEM-EDS, ICP-MS, 화학습식분석법 등을 이용하였다. 최상품 자기는 매우 정선된 수비과정을 거쳤으며, 알바이트가 풍부한 도석 원료를 사용하였다. 티타늄이 포함되지 않고, 0.5~0.8wt.% 정도의 매우 낮은 철함량을 포함하고 있는 것이 특징이다. 유약 성분은 용제 함량을 낮추었으며, 라임이 10% 정도로 낮고, 알칼리의 비율이 높은 라임-알칼리 계열로 고화도 번조에 알맞게 조절하였다. 가마에서의 번조과정에서도 보다 강한 환원분위기로 제어한 것으로 파악되었다. 번조분위기를 완벽하게 조절할 수 있게 됨에 따라 태토 내에 포함되어 있는 철성분에 의해 태토색이 어두워지는 것을 방지하고 최대한 백색도를 높힐 수 있었던 것으로 보인다. 또한, 분석 결과를 통하여 태토의 원료 선택과 수비법, 그리고 유약의 제조기술의 적용에 있어서도 양식적인 구분에 따라 의도적인 차이를 두었음이 확인되었다. 즉, 자기 제작에 있어서 원료의 선정부터 마지막 번조과정에 이르기까지 차별화된 제작시스템을 적용함으로써, 소비주체에 따른 생산품의 질적 다양화가 이루어졌으며, 보다 효율적인 운영을 하였던 것으로 판단된다.

일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: KCS3-5

발표분야: Chemistry for Conservation of Cultural Properties

발표종류: 심포지엄, 발표일시: 목 15:20, 좌장: 도진영

Stability tests of citric acid with ancient pottery for cleaning inorganic stains

박대우, 장성윤

국립문화재연구소 복원기술연구실

This study investigate on the stability of citric acid which used for removal of iron stains on ancient pottery. The elution characteristics of major elements (Si, Al, Fe) and difference of colours on pottery were observed after soaking test with citric acid. Major elements were eluted 0.237ppm to 28.639ppm from the samples of Tangjeon, Asan when soaking with 0.25M citric acid for 130minutes. This elution characteristics increased according to the absorption of samples. The slope of elution is not proportional until the absorption of 12%, but it starts to grow in geometrical progression over 12%. Also the characteristic of elution is related to the firing characteristics of pottery. The ancient pottery with Mullite which was created at high fired progress has absorption under 12% and doesn't appear the characteristic of elution, but over 12% showed distinctly. As color difference(ΔE_{ab}^*) of pottery is observed under 4, the soaking of citric acid for 130 minutes does not affect on stability of high fired samples. However, it is necessary to be careful on the low fired pottery which have deteriorated surface.

일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: **KCS3-6**

발표분야: Chemistry for Conservation of Cultural Properties

발표종류: 심포지엄, 발표일시: 목 16:00, 좌장: 도춘호

A Study of the Chemical Composition of Korean Traditional Ceramics : Celadon and Koryo Whiteware

안상두, 고정신

중앙대 화학과

Scientific studies of traditional Korean shards commenced in the United States and Germany in the 1980s, and studies within Korea began in the 1990s. From analysis of a large systematically collected dataset, the composition of porcelain produced during the Koryŏ dynasty, including 21 celadon and 10 whiteware groups, was characterized and compared with that of Chinese ceramics. The average composition of the body and glaze of several shards (usually three to five) from each group was determined, enabling comparisons between groups. The results show that the majority of groups were derived from mica-quartz porcelain stone, which was commonly used in Yuezhou, Jingdezhen, and other southern Chinese kilns. The composition of glazes includes clay and flux components; the latter were typically wood ash and limestone, initially as burnt but later as crushed forms. The earliest of the Kangjin glazes contained substantially less titanium oxide than did the Yuezhou glazes, which were typically formulated from body material and wood ash. The present study provides a comparative framework for the growing number of analytical investigations associated with excavations occurring in Korea.

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장소: 제주ICC

발표코드: KCS3-7

발표분야: Chemistry for Conservation of Cultural Properties

발표종류: 심포지엄, 발표일시: 목 16:20, 좌장: 도춘호

Reconstructing Dietary Patterns of the Historical Populations in Korea Using Stable Isotope Analysis

강소영

국립문화재연구소 보존과학연구실

Overall understanding life style of social, regional and temporal characterization of the Joseon people, carbon and nitrogen stable isotope analysis was performed on 157 human skeletal remains from various archaeological sites in Korea. Stable isotope values range mainly from -20.0‰ to -18.8‰ for carbon and from 8.8‰ to 11.2‰ for nitrogen, indicating Joseon people consumed mainly C₃ plant. Human skeletons from lime-layered tomb has relatively more elevated mean $\delta^{13}\text{C}$ and $\delta^{15}\text{N}$ values than them from tomb. These results suggested that social organization is one of the decisive factors in determining dietary patterns of the Joseon period.

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장소: 제주ICC

발표코드: KCS3-8

발표분야: Chemistry for Conservation of Cultural Properties

발표종류: 심포지엄, 발표일시: 목 16:40, 좌장: 도춘호

고대 안료의 납동위원소비 분석방법 연구

이한형, 한민수, *정연중

국립문화재연구소 보존과학연구실 *한국기초과학지원연구원 환경과학연구부

납을 주성분으로 하는 안료 중 고대로부터 사용되어온 안료는 연분, 황단, 연단 등이 있다. 이들 안료는 천연에서 채취되기도 하지만, 기원전부터 인공적 제조방법이 전해지는 대표적인 고대 인공 안료이다. 연분의 제조에는 납이 이용되는데, 납의 동위원소비는 현재 청동유물의 산지추정 연구에 활발하게 이용되고 있다. 따라서 청동유물과 마찬가지로 고대 회화나 단청 등에서 발견되는 이들 납 포함 안료의 납동위원소비 분석은 고대 안료의 교역경로에 대한 정보를 제공할 수 있다. 그러나 고대 회화나 단청 등에 적용된 안료는 많은 경우 여러 색상의 안료가 층을 이루는 다층박막형태를 띠고 있으며, 채색시 사용된 고착제의 열화로 매우 부서지기 쉬운 상태로 존재하게 된다. 따라서 분석을 위한 시료채취가 어려우며, 인접한 안료층에 의한 오염의 영향을 배제할 수 있는 방안이 요구된다. 본 연구에서는 TIMS, HR-SIMS, LA-ICP-MS 등을 이용하여 납 함유 안료시료의 납동위원소비 분석을 시도하고, 각 분석법에 따른 인접 안료층의 오염 배제 가능성을 검토하였다. 먼저 납을 주성분으로 하는 안료로서 백색인 연분($2\text{PbCO}_3 \cdot \text{Pb(OH)}_2$)과 적색인 연단(Pb_3O_4)을 선정하고, 순수한 분말 상태의 안료에 대하여 TIMS를 이용하여 납동위원소비를 분석하였다. 다음으로 납동위원소비가 확인된 이들 안료를 고착제와 배합하여 다층구조를 이루는 채색시료를 제작하고, 채색시료에서 소량의 채색층을 채취하여 TIMS, HR-SIMS, LA-ICP-MS를 이용한 분석을 수행하였다. 그 결과 TIMS의 경우 시료채취 시 인접층에 존재하는 안료에 의한 오염을 배제하기가 매우 어려웠으며, HR-SIMS와 LA-ICP-MS의 경우 안료 층의 두께가 비교적 두꺼운 시료에 대하여 인접안료의 영향이 배제된 결과를 얻을 수 있었다. 그러나 얇은 채색시료의 경우 인접 안료층의 영향을 완전히 배제하기 위하여 분석 시료의 단면 가공 방법과 분석 spot의 크기 조정 등의 연구가 지속적으로 요구된다.

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장소: 제주ICC

발표코드: KCS3-9

발표분야: Chemistry for Conservation of Cultural Properties

발표종류: 심포지엄, 발표일시: 목 17:00, 좌장: 도춘호

비파괴분석법을 이용한 백자의 생산지 분류

김규호, 김나영

공주대 문화재보존과학과

본 연구는 에너지분산형 X-선형광분석기(EDXRF, Energy Dispersive X-Ray Fluorescence Sequential Spectrometer, Model : Seiko Ins. SEA 2220A, Japan)를 이용한 비파괴 분석법으로 기계유씨 묘에서 출토된 백자의 생산지를 추정해 보고자 하였다. 형태적 특성에서 기계유씨 묘 백자는 인접한 부여 정각리 갯점골 가마터 출토 백자와 기형, 제작 방법, 태토의 색상 등에서 유사성이 제기된 바 있다. 제작 산지는 부여 정각리 갯점골, 청양 광대리 및 대박리, 하동 백련리, 사천 사촌리 가마터 출토 백자와 비교한 결과에서 기계유씨 묘 출토 백자는 다른 지역에 비하여 부여 정각리 갯점골 백자와 상관성이 높게 측정되었다. 측정 방법은 국외에서 선행된 흑요석, 토기, 자기에 대한 산지 연구 방법을 기초하여 K, Ca, Ti, Mn, Fe, Rb, Sr, Y, Zr, Ba 등 10 개 원소를 측정하였다. 전압, 필터, 전류, 시료의 전처리, 측정 시간 등 측정 조건은 표준시료를 측정하여 설정하고 동일한 연구 도편을 중성자방사화 분석법으로 측정하여 X-선형광분석기를 활용한 비파괴 분석법의 재현성 및 신뢰성을 검토하였다. 이와 같은 비파괴분석법을 활용한 도자기의 특성 분석은 앞으로 가마터별 분석 자료가 축적되면 백자의 산지 분류에 대한 과학적 기초 정보를 제공할 수 있을 것으로 생각된다.

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장소: 제주ICC

발표코드: KCS3-10

발표분야: Chemistry for Conservation of Cultural Properties

발표종류: 심포지엄, 발표일시: 목 17:20, 좌장: 도춘호

석조문화재 표면에 형성된 칼슘염의 생성메커니즘과 염풍화시험에 의한 작용성 연구-경주지역 석조문화재를 중심으로-

도진영

경주대 문화재보존학과

경주지역 석조문화재의 표면에는 황산칼슘 및 탄산칼슘을 대표로 하는 칼슘염이 다량 형성되어 있다. 이들의 형성경로와 석조문화재의 보존에 미치는 영향을 살펴보기 위하여 소량의 시료를 석조문화재로부터 채취하여 XRF 에 의한 화학성분, IC 에 의한 수용성이온성분, XRD 에 의한 광물성분을 분석하였고, 실체현미경과 전자현미경을 통하여 미세조직을 관찰하였다. 경주지역 석조문화재의 구성 석재는 화강암과 석영안산암 및 안산암 등으로 밝혀져, 표면에 형성된 칼슘염의 주 화학성분인 Ca 와 S 의 기원물질이 되지 않으며, 과거에 사용된 보수물질이 다량의 Ca 을 함유하고 있음이 분석되어 주 기원물질로 파악되었다. 석조물 표면에서 검출되는 S 의 주기원물질은 보수물질이 함유하고 있는 S 성분이었으며, 석조물 주변 공기질의 분석결과 대기중의 S 함유물질의 영향도 있음을 밝혔다. 칼슘염의 용해량은 Ca^{2+} 약 27wt.%, SO_4^{2-} 는 47wt.%에 달하는 값으로 측정되어 빗물이 직접 닿지 않는 석조물 표면에서 재결정화과정이 반복된다. 칼슘염은 전자현미경하에서 관찰한 결과 10 μm 크기의 침상 또는 판상의 결정을 이루고 있으며, $\text{Ca}(\text{OH})_2$, 방해석(CaCO_3)과 석고($\text{CaSO}_4 \cdot 2\text{H}_2\text{O}$)성분인 것으로 밝혀졌다. 칼슘염이 형성되어 있는 부위에서 집중적으로 박리현상과 입상분해현상이 관찰되었다. 칼슘염을 이용한 염풍화시험결과, $\text{CaSO}_4 \cdot 2\text{H}_2\text{O}$ 는 낮은 용해도로 인하여 상대적으로 암석의 내부로 깊이까지 들어가서 집적되고, 집적되는 부위에서 박리현상이 발생하는 것으로 나타났다.

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장소: 제주ICC

발표코드: KCS4-1

발표분야: KCS School - 플라스마기술과 산업적 응용

발표종류: 심포지엄, 발표일시: 목 14:00, 좌장: 한승희

증착 및 식각 공정용 플라스마 장비의 디자인

주정훈

군산대 신소재공학과

재료 공정에 사용되는 플라스마의 역할은 사용하는 가스의 종류에 따라서 물리적 스퍼터링, 이온 보조 식각, 라디칼 증착, 이온 증착, 라디칼 치환 등으로 나눌 수 있다. 이 중 물리적인 효과가 우선시 되는 공정에는 이온의 밀도가 높고 운동 에너지의 조절이 용이한 고진공 고밀도 플라스마가 유리하다. 대표적인 예는 고밀도 유도결합 플라스마 시스템이며 반도체의 식각, 증착, 도핑, 다이싱(dicing) 공정에 이용되고 있다. 이온의 과도한 충돌이 오히려 격자 결함이나 화학 결합의 손상을 유발하는 경우에는 플라스마 전위가 낮고 밀도만 높은 저진공 고밀도 플라스마 공정이 유리하다. 본 세미나에서는 플라스마가 담당하고 있는 증착 및 식각 공정의 원리가 무엇인지 해석하고 이와 동등한 기능을 보다 저렴하고 대용량화 하기 위한 장비 개발의 원리적 접근 방법 및 이를 위한 화학적 지식의 필요성에 대해서 논의한다. 플라스마 공정의 해석과 이를 응용한 산업용 장비의 개발에 있어서 필수적인 공정 및 장비의 수치 모델링 기법과 위의 사례에 사용된 Ar, N₂ 및 CF₄ gas 에 대한 플라스마 화학 반응에 대한 분석을 통하여 플라스마 내에서 전자의 충돌에 의해서 유발되는 공간 이온화, 해리, 해리 이온화, 여기 반응의 특성과 이들 라디칼과 이온, 전자들이 재료 표면에서 일으키는 여러 가지 표면 반응에 대한 모델을 소개하고 식각, 증착 등에서 이들이 플라스마 내의 공정 변수 (전력, 압력, 전위)에 의해서 어떤 메커니즘으로 작용을 하고 있는지 소개하고 최근 수행되고 있는 300 mm wafer 처리용 장비의 개발에 적용된 수치 해석 결과를 소개한다.

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장소: 제주ICC

발표코드: **KCS4-2**

발표분야: KCS School - 플라스마기술과 산업적 응용

발표종류: 심포지엄, 발표일시: 목 14:30, 좌장: 한승희

Research Activities on PIII&D (Plasma Immersion Ion Implantation and Deposition) Technology at KIST

한승희

KIST 특성분석센터

PIII&D (Plasma immersion ion implantation and deposition) technology is a very promising surface modification technology to improve the materials surface properties. In PIII&D, plasma immersion ion implantation technique, which is a very effective way to implant gaseous ions into the materials surface, is combined with thin film deposition technique such as magnetron sputtering. Thin films can be simultaneously modified by high-energy ion bombardment during deposition to improve the film properties. Furthermore, by operating the magnetron sputter deposition in high-power pulsed mode synchronized with the high voltage negative pulse bias that is applied to the substrate, non-gaseous ions such as metallic ions can be effectively implanted into the substrate owing to the highly ionized plasma state of sputtered target atoms. At KIST, PIII and PIII&D technique have been applied to numerous fields for many years to modify materials surface, which includes improvement of wear property, shallow junction doping, polymer surface modification, application to SOI wafer manufacturing, quantum dot formation, application to artificial hip joint materials, etc. In this talk, the research activities and experimental results on PIII&D technology will be shown and discussed.

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장소: 제주ICC

발표코드: KCS4-3

발표분야: KCS School - 플라스마기술과 산업적 응용

발표종류: 심포지엄, 발표일시: 목 15:00, 좌장: 한승희

저온 대기압 플라스마의 생의학 응용

서영식

포항공과대 전자전기공학과

대기압 플라스마는 다양한 생의학 분야(암치료, 치아미백, 상처치유, 멸균)에 높은 적용 가능성을 보여준다. 그 이유는 대상 물질에 열 손상을 최소화할 수 있는 저온 처리특성과 생의학 분야에 중요 인자인 활성종을 다량으로 발생시키기 때문이다 [1-2]. 이와 더불어, 대기압 플라스마는 고가의 진공 장비를 필요로 하지 않고 소규모의 전력공급 장치로 구동이 가능하기 때문에 저비용, 소형화 특성을 보유하고 있어 산업화에 강점을 갖는다. 다양한 생의학 응용 분야 중 대기압 플라스마의 강력한 멸균 특성 연구가 먼저 시작되었지만, 현재 큰 관심을 끄는 분야는 세포의 사멸 유발 또는 성장 촉진과 연관이 있는 암치료와 상처치유이다 [3-4]. 피부암 세포를 대상으로 한 실험을 위해 20 kHz 정현파로 구동되는 플라스마 장치를 고안하였고 플라스마 효과를 암세포에만 선택적으로 증대시키기 위해 항체-금나노입자 중합체를 암 세포에 주입시켰다. 그 결과 항체-금나노입자 중합체에 플라스마를 처리한 경우 피부암 세포의 사멸율은 74%로서 대조군에 비하여 2 배에서 5 배까지 증가하였다. 또한 플라스마 처리는 세포의 DNA 에 손상을 유발시키며 이를 통해 암세포의 자멸사를 유도한다 [5]. 플라스마는 세포의 성장 촉진에도 영향을 미쳤으며, 플라스마 처리 후 심한 상처가 빠르게 치유되는 것이 입증되었다 [6]. 현재 세포에 영향을 미치는 플라스마의 정확한 성분에 관한 연구가 다양하게 행해지고 있다. 치아 미백에 대한 대기압 플라스마의 적용은 최근 급부상하고 있다 [7-9]. 대기압 플라스마를 기존 치아 미백에 사용되는 과산화수소와 함께 발치된 치아에 10 분간 처리하였을 때 미백제만을 사용한 경우에 보다 치아의 색상 변화가 2 배 이상 증가하였으며, 치아 표면의 단백질도 깨끗이 제거되었다. 또한 저주파 플라스마보다 많은 강점을 갖는 고주파 플라스마를 활용하여 지혈과 충치균을 처리하였으며 그 탁월한 효과가 입증되었다 [10-12]. 혈액 응고 실험을 위해 30 초 정도 짧은 플라스마 처리만으로도 자연 응고에 비해 지혈 효과가 뛰어났으며, 충치를

발생시키는 대표적인 구강균인 *S.mutans* 을 대상으로 한 실험에서 30 초 미만의 처리로 멸균의 지표인 10^{-6} 만큼의 멸균능력을 확인하였다. 대기압 플라즈마의 생의학 응용 기술의 최적화를 위해서는 세포로 대변되는 처리물질과 대기압 플라즈마의 상호 관계, 여러 조건하에서의 대기압 플라즈마의 특성 변화, 응용별 기저 기작에 대한 이해와 연구가 필요하며, 시뮬레이션의 활용과 다학제간 협력연구가 중요하다.



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장소: 제주ICC

발표코드: **KCS4-4**

발표분야: KCS School - 플라스마기술과 산업적 응용

발표종류: 심포지엄, 발표일시: 목 15:50, 좌장: 주정훈

PGV (Plasma Gasification and Vitrification) 공정을 이용한 청정 합

성가스의 생산과 활용

황순모

GS플라텍

플라즈마 토치를 이용하여 폐기물이나 저급연료를 처리하면서 동시에 청정한 합성가스를 생산하여 활용할 수 있는 수단으로 PGV (Plasma Gasification and Vitrification) 공정이 개발되었다. 비교적 단순하고 안정적인 과정을 통해 친환경적인 동시에 경제적으로 합성가스를 생산할 수 있으며, 이를 통해 스팀과 전기 및 고순도 수소 등 다양한 형태의 에너지 자원을 높은 효율로 회수해 낼 수 있다. 질소 및 황 산화물과 다이옥신 등 유해 물질의 발생 및 배출억제와 제어에 관해 언급하고, 운전중인 상용시설의 실제 측정결과와 비교하며, PGV 공정의 개발현황과 향후 추진방향 및 응용분야에 대해 소개한다.

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장소: 제주ICC

발표코드: KCS4-5

발표분야: KCS School - 플라스마기술과 산업적 응용

발표종류: 심포지엄, 발표일시: 목 16:20, 좌장: 주정훈

Water treatment by various plasmas

이봉주

국가핵융합연구소 융복합플라즈마 연구센터

수처리를 위한 다양한 플라즈마 발생이 연구되었다. 용존 오존을 높이기 위한 시도로 기액방전을 시작으로 현재는 지표수와 바닷물에서 수중방전을 연구 중이다. 수중방전은 다양한 라디칼을 직접 물 속에서 발생시키기 때문에 수처리 공정에 다양한 응용이 가능하다. 특히, 최근에 선박평형수 등의 살균이 국제적인 이슈가 되고 있고, 2017년까지는 모든 선박에 살균을 위한 수처리 설비가 의무화된다. 염분이 있는 수체에서의 방전공정을 연구하고 이를 수처리공정에 적용할 수 있는 방법에 대해 연구하였다. 해수의 경우 전도도가 53mS로 자유로운 전하의 이동이 가능하기 때문에 일반적인 민물방전의 전원과 전극 등으로는 방전을 할 수 없다. 이에 세라믹과 금속의 이중구조로 되어 있는 모세관전극을 개발하여 전도성이 있는 수체에서의 방전을 이루었다. 전원장치로는 60 Hz, 380 V를 1 차측에 인가하여 2 차측에서 약 3 kV, 10 kW의 파워가 발생하는 12 위상차 교류전원장치를 개발하여 사용하였다. 모세관 내부에 전압이 인가되면 전류가 발생하여 joule heating에 의하여 모세관 내부에 기포가 형성된다. 이 때, 전류의 단락이 이루어지면서 고전압쪽에 전하가 축적되며 기포내부의 E-field가 상승한다. 이후 기포 내에서 방전이 개시되며 각종 라디칼을 생성한다. 방전에 의해 생성되는 산화제로는 오존, OH 라디칼, 과산화수소 등이 있으며, 해수에서는 Cl⁻의 결합에 의하여 Cl₂ 가스가 발생한다. 약 30,000 J/L의 체적에너지에 대하여 생성되는 총염소의 농도는 2.5 mg/L이다. 수중방전의 적용대상으로 선박평형수, 멤브레인과의 결합, 용존기포부상법을 선정하여 적용가능성을 연구하였다. 먼저 선박평형수 살균처리를 위해 해수의 처리유량을 20 lpm으로 유지하고 대장균, 바실러스, 조류(테트라셀미스) 등을 투입하여 전극 12 개가 삽입된 12 위상차 플라즈마 반응기를 통과시켰더니, 약 30,000 J/L의 체적에너지에 대하여 1일 후의 살균력이 각각 99.99, 99.99, 99.9 %의 살균력을 나타내었다. 이는 국제해사기구에서 권장하는 살균수준인 99.9%를 초과하는 수치이다. 최근에는 수중방전기에 가스를 주입하는 방식으로

같은 결과를 1/10 수준의 체적에너지로 가능할 수 있음을 보고하였다. 플라즈마를 이용한 해수살균공정의 안정적 운전을 위해 후단에 UF 멤브레인을 추가하여 잔류생존 미생물을 제거할 수 있다. 이를 위해 플라즈마가 후단의 멤브레인 운전에 미치는 영향을 평가하였다. 카울린과 탄산칼슘을 오염원으로 각각 투입하여 멤브레인으로 처리를 하였을 때, 방전 직후 멤브레인에 걸리는 막간압력차가 약 30% 감소하였는데, 이는 막에 형성된 파울링이 방전에 의해 제거된 것으로 평가할 수 있다. 수중방전은 다양한 산화제를 생성함과 동시에 미세기포를 발생시키는데 이는 수중유기물의 부상분리에 적용될 수 있다. 방전모세관전극의 내부직경을 1 mm 로 유지하고, 60Hz, 교류전원으로 방전한 결과 평균입경 44 μm 의 기포를 발생시켰고, 이는 일반적으로 용존공기부상법에 사용되는 기포의 크기와 일치한다.



일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: KCS4-6

발표분야: KCS School - 플라스마기술과 산업적 응용

발표종류: 심포지엄, 발표일시: 목 16:50, 좌장: 주정훈

Thermal plasma synthesis of nano-composite materials for industrial applications

서준호

전북대 고온플라즈마응용연구센터

최근, 다양한 산업적 응용을 위해 활발하게 적용되고 있는 열플라즈마를 이용한 나노분말 합성법에 대해서 소개한다. 높은 온도 ($>5000\text{ K}$) 와 급랭율 ($> 10^6\text{K/s}$)을 제공할 수 있고, 산화, 환원 및 불활성 분위기의 자유로운 제어가 가능한 열플라즈마의 전형적 특징은 50~100 nm 크기의 금속, 세라믹, 유리 및 복합분말 합성에 있어 액상법 등 재래식 방법에 비해 다양한 이점을 제공할 수 있다. 대표적인 예로서, MLCC 등 전자산업용 금속, 세라믹 및 유리 나노 분말 합성에 활용될 수 있으며, 희유금속 저장재료, 메탄 개질용 촉매재료 및 디스플레이용 고성능 재료 개발에 있어서도 열플라즈마의 고유 장점이 타 방법에 비해 우수한 기술 경쟁력을 가져다 줄 것으로 기대된다. 이와 같은 응용분야를 중심으로 열플라즈마를 이용한 나노분말 합성법의 이론 및 역사적 배경, 장치 구성 방법과 최근 전북대학교 고온플라즈마센터에서 수행한 합성분말 특성 분석 결과 등에 대해 발표하고자 한다.

일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: **INOR.O-1**

발표분야: General Oral Presentation

발표종류: 구두발표, 발표일시: 금 13:30, 좌장: 오문현

Application of NHC-Organometallics for Functional Materials

손성욱

성균관대 화학과

N-Heterocyclic carbene (NHC) has been extensively studied in the field of organometallics as a new coordination mode comparable to the conventional phosphine ligands. The NHC coordination mode can be generated via the abstraction of protons from disubstituted imidazolium salts. Typically, NHCs are capable of coordinating with a wide range of transition metals and diverse studies for applications of NHC-metal complexes have been conducted. In this paper, the application of NHC-chemistry in synthesis of diverse functional materials will be presented.

일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: **INOR.O-2**

발표분야: General Oral Presentation

발표종류: 구두발표, 발표일시: 금 14:00, 좌장: 오문현

Advances with the Zintl Phases Containing an Incommensurately Modulated Structure

유태수

충북대 화학과

The Zintl-Klemm formalism has enjoyed tremendous success for rationalizing numerous network- and cluster-based structures involving main group elements. As research continues to explore the applicability of this potentially predictive concept, developments in theoretical and computational chemistry allow the study of larger and heavier molecular and solid-state building blocks to test this powerful formalism semi-quantitatively, as well as improved handling of interatomic interactions involving widely disparate elements. Inherent in the Zintl-Klemm formalism is a coexisting tension between anisotropic, covalent bonding interactions, and isotropic, ionic, or metallic bonding forces collected in a system whose equilibrium volume is governed by atomic sizes via core repulsions. One example is the species related to MgB_2 , which are rationalized using the Zintl-Klemm concept, engendered renewed enthusiasm and interest during the past decade due to the discovery of an unusually high superconducting transition temperature at 39 K in MgB_2 itself. CaAlSi with 9 valence electrons is one of those related species, and with respect to the Zintl-Klemm formalism, 9 e^- graphite sheet is somewhat electron-rich. Thus, the $\text{RE}(\text{M}_{1-x}\text{M}'_x)_2$ system creates a fertile garden of compounds to examine the inter-relationships among atomic sizes, valence electron concentrations as well as role of cations on structure-property relationships in Zintl phases. Here, two series of Zintl compounds will be discussed in terms of experimental and theoretical investigations: (1) three isoelectronic compounds EuGaTt ($\text{Tt} = \text{Si}, \text{Ge}, \text{Sn}$) with 9 e^- and (2) the $\text{EuZn}_{1-x}\text{Ge}_x)_2$ ($0 \leq x \leq 1$) series including an incommensurately modulated structure at $x = 0.75$, and discuss their different structure types and the driving force determining those structures using various analyses based on quantum-theoretical calculations. Physical properties of those materials will also be discussed.

일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: **INOR.O-3**

발표분야: General Oral Presentation

발표종류: 구두발표, 발표일시: 금 14:20, 좌장: 오문현

Development of High Functional Resin Coated Electrogalvanized Steel Sheet for Digital TV Panel

조두환

(주)포스코 기술연구원 표면처리연구그룹

Recent digital TV industry has drastically been moving the illuminating system, from PDP and LCD to LED to provide high-definition image. Due to strong competition, the TV makers would like to reduce production cost by using low-priced materials such as steels instead of aluminum and plastic materials *etc.*. In this paper we have developed new low-priced electrogalvanized steel sheet, which is coated black colored high functional resin composite, is substitute high-priced PCM steel and plastic for rear cover panels in the digital TV. The coating resin composite was prepared by ball-milling procedure the mixture solution that consist of high solid polyester resin, melamine hardner, black pigment, and additives. the composite solution was coated on the steel sheet by using roll coater via induction curing furnace. although the coated layer has 10 micrometers thickness, comparative conventional PCM steels having 25 micrometers, exhibits excellent quality to use rear cover panel. The new steel sheet was applied to get quality certification from customer(Samsung & LG electronics). Detailed discussion will be present including composite preparation, roll coating technology, induction curing, and quality evaluation.

일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: **INOR.O-4**

발표분야: General Oral Presentation

발표종류: 구두발표, 발표일시: 금 14:40, 좌장: 오문현

Ionothermal Synthesis of Porous Carbon Materials Using Fluidic Carbon Precursors

이제승

경희대 화학과

Porous carbon materials are widely applied to separation, supporter, energy storage, and energy conversion for their huge surface areas, high physical and chemical stability, and high electric conduction. New synthetic strategy of porous carbon materials which is not needed template have been developed because conventional hard or soft template methods are suffering the difficulty of post-treatments or the limitation of surfactants and the difficulty of carbon coating on the substrates. Specific task ionic liquids containing cross-linkable functional groups on cation or anion were successfully carbonized under ambient pressure for their negligible vapor pressure and high thermal stability. The surface area could be controlled by the size of counter ion. Various shaped substrates could be carbon-coated successfully.

일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: INOR.O-5

발표분야: General Oral Presentation

발표종류: 구두발표, 발표일시: 금 15:00, 좌장: 오문현

A Novel Approach for the Investigation of Hydrogen Storage Mechanism - In-situ Neutron Scattering and In-situ Raman Scattering.

최용남, 이희주

한국원자력연구원 중성자과학연구부

Hydrogen has been considered as an alternative for the future energy source. However, though a lot of efforts to explore high efficiency storage materials at feasible conditions were done, it seems to be at a stand-still unless there appears a novel breakthrough. Most of the tries on the hydrogen storage works were based on the design-synthesis-measurement(specific surface area and $c(P,T)$). Less tries on the measurements of the structure and/or the dynamics of the hydrogen and sorbing materials during the sorption and desorption processes have been reported. Understanding of the sorption/desorption mechanism is an essential factor prior to the design of a new material. To investigate the mechanism for the hydrogen storage we have recently established an in-situ neutron diffraction sample environment which enable us to obtain the neutron diffraction patterns and the adsorption capacity of the state (P and T). And we are now trying to construct a new and powerful experimental platform, 'In-situ Combined Scattering (neutron diffraction + Raman + $c(P,T)$) Apparatus', which may give us more insightful information on the hydrogen storage and it is expected to be operational in this year. Some results from the in-situ neutron diffraction experiment will be introduced and discussed.

일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: INOR.O-6

발표분야: General Oral Presentation

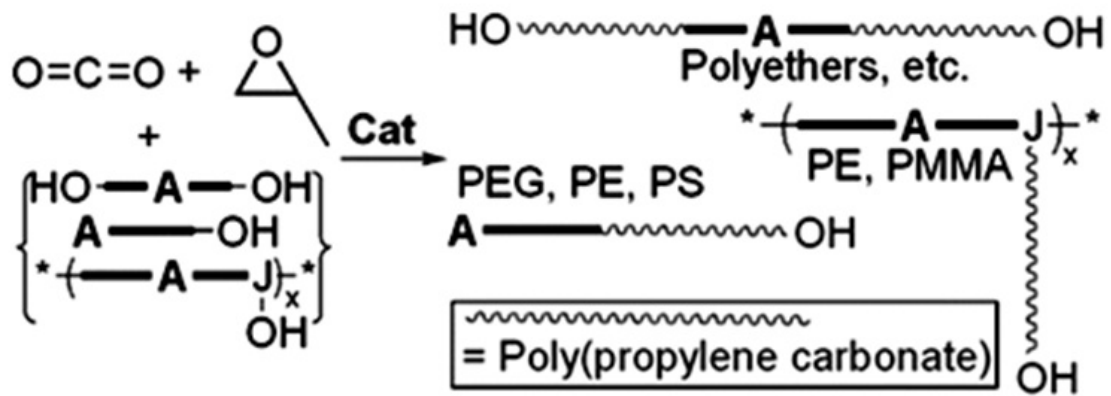
발표종류: 구두발표, 발표일시: 금 15:25, 좌장: 나명수

Immortal CO₂/Propylene Oxide Copolymerization ; Architecture of Various Block Copolymers and Connection of Polymer Chain Using a Highly Active Catalyst

Anish Cyriac, 이상환, 이분열

아주대 분자과학기술학과

A highly active and relatively cheap catalyst for CO₂/propylene oxide (PO) copolymerization is developed (TOF 15000 h⁻¹). It was revealed that the high activity of these kind of complexes, due to an unusual binding mode of a Cobalt(III) complex prepared from a Salen-type ligand tethered by four quaternary ammonium salts. This catalyst preserves an excellent catalytic performance even in the presence of a large amount of protic compounds which enables us to efficiently perform "immortal polymerization" in CO₂/propylene oxide copolymerization. Precise control of molecular weight is achieved by feeding various protic compounds such as adipic acid, which resulted in the formation of low molecular weight poly(propylene carbonate)-diol (PPC-diol). By feeding bulk polymer contains OH or COOH in immortal polymerization, we have demonstrated block and graft copolymerization. When a small amount of vinylcyclohexene dioxide is additionally added in CO₂/PO copolymerization some of the polymer chains are connected consequently resulting an increased molecular weight up to $M_w = 60600$ and broad molecular weight distribution. The same chain-connecting process is also applicable in the presence of chain transfer agent, tricarballic acid, 1,2,3,4-butanetetracarboxylic acid, or adipic acid, although a higher amount of diepoxide is needed. The poly(propylene carbonate)-*block*-poly(ethylene glycol) copolymer, which is obtained by feeding poly(ethylene glycol)-OH as a chain transfer agent, becomes tough in the tensile property and shows a high shear sensitivity in the rheological property when some chains are connected using diepoxide.



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장소: 제주ICC

발표코드: INOR.O-7

발표분야: General Oral Presentation

발표종류: 구두발표, 발표일시: 금 15:30, 좌장: 나명수

Structure, Interconversion, and Reactivity of Peroxo, Hydroperoxo, and Oxo Ligands in a Nonheme Iron Complex

전수진, *남원우

이화여대 바이오 융합과학과 *이화여대 화학과

Iron-oxygen species, iron(III)-peroxo, iron(III)-hydroperoxo, and iron(IV)-oxo, are key intermediates often detected in the catalytic cycles of dioxygen activation by heme and nonheme iron enzymes. Here, we report for the first time the high-resolution crystal structure of a mononuclear side-on iron(III)-peroxo complex, $[\text{Fe(III)(TMC)(OO)}]^+$ (TMC = 1,4,8,11-tetramethyl-1,4,8,11-tetraazacyclotetra-decane). The high-spin iron(III)-peroxo complex is converted to a low-spin iron(IV)-oxo complex, $[\text{Fe(IV)(TMC)(O)}]^{2+}$ via a high-spin iron(III)-hydroperoxo complex, $[\text{Fe(III)(TMC)(OOH)}]^{2+}$. Relative reactivity studies performed with the iron(III)-peroxo, iron(III)-hydroperoxo, and iron(IV)-oxo species reveal that the iron(III)-hydroperoxo complex is the most reactive of the three in the deformylation of aldehydes (i.e., nucleophilic reaction) and has a similar reactivity to the iron(IV)-oxo complex in C-H bond activation of alkylaromatics (i.e., electrophilic reaction). The latter results demonstrate that iron(III)-hydroperoxo species are viable oxidants in the electrophilic and nucleophilic reactions by iron-containing enzymes.

일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: INOR.O-8

발표분야: General Oral Presentation

발표종류: 구두발표, 발표일시: 금 15:35, 좌장: 나명수

Spin canting-dependent magnetic variations of one-dimensional Mn(III) compounds bridged by a single azide

윤정희, 홍창섭

고려대 화학과

Single chain magnets (SCMs) are of importance due to their unusual physical properties and potential applications in information storage. The strategies used frequently are to devise one-dimensional (1D) chains with ferromagnetic, ferrimagnetic or canted antiferromagnetic coupling. Azide is an efficient ligand for building up diverse structural patterns and being able to predict magnetic properties depending on the binding mode; the end-on mode transmits a ferromagnetic interaction and the end-to-end mode mediates antiferromagnetic coupling. One-dimensional polymer $[\text{Mn}(\text{5-Brsalpn})(\text{N}_3)]$ (1) linked by azide in end-on mode and three compounds in end-to-end mode $[\text{Mn}(\text{3-MeO-salpn})(\text{N}_3)] \cdot 0.5\text{AClO}_4$ [$\text{A}^+ = \text{Na}^+$ (2), K^+ (3), Rb^+ (4)] have been successfully obtained and structurally characterized. 1 and 2 displayed atypical antiferromagnetic couplings and field-induced two-step magnetic transitions, while compounds 3 and 4 show a field-induced metamagnetic transition. Remarkably, compounds 1, 2 and 3 exhibit SCM properties with slow relaxation of the magnetization. The spin-canted phenomenon is found to play a pivotal role in establishing slow magnetic relaxation, which proves to be a rational approach to attain SCMs.

일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: INOR.O-9

발표분야: General Oral Presentation

발표종류: 구두발표, 발표일시: 금 15:40, 좌장: 나명수

Photocatalytic Activity of Pt Nanoparticles for Visible Light-Driven Production of NADH

김가영, *김진아, **차미선, ***Wu Qiong, ****김진홍

이화여대 화학나노과학부 *이화여대 무기화학 **이화여대 화학나노과학과 ***이화여대 나노과학부 ****이화여대 화학과

As fossil fuels continue to be depleted, tremendous and numerous efforts have been made for the development of alternative energy supplies. One topic that has fascinated scientists is the notion that radiant electromagnetic energy is transformed by photochemical systems to yield chemical energy in the form of a reducing potential, such as dihydronicotinamide adenine dinucleotide(NADH). NADH is used as a cofactor in various biological reactions performed by many redox enzymes. Because the cofactor, which is used in stoichiometric amounts in biological reactions, is expensive, the development of efficient systems that can carry out solar energy capture and conversion is of substantial interest for NADH regeneration. Furthermore, visible light-driven systems have attracted significant interest because 46% of total solar light is within the visible range. In studies that mimic natural photosynthesis, a system containing three independent components, a photosensitizer, electron relay, and catalyst, has been used with a sacrificial electron donor. In this study, we created a novel system for the photocatalytic generation of NADH from aqueous protons using only Pt nanoparticles without and additional photosensitizer, electron relay, and homogeneous organometallic catalyst. We found the irradiation of the Pt nanoparticle solution with visible light converts NAD⁺ to NADH with a high yield of 86% in the presence of triethanolamine as a sacrificial electron donor. The rate of NADH photogeneration depended on the concentration of PtNPs and TEOA. The rate of NADH generation also increased with NAD⁺ concentration at low values and reached a plateau.

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장소: 제주ICC

발표코드: **INOR.O-10**

발표분야: General Oral Presentation

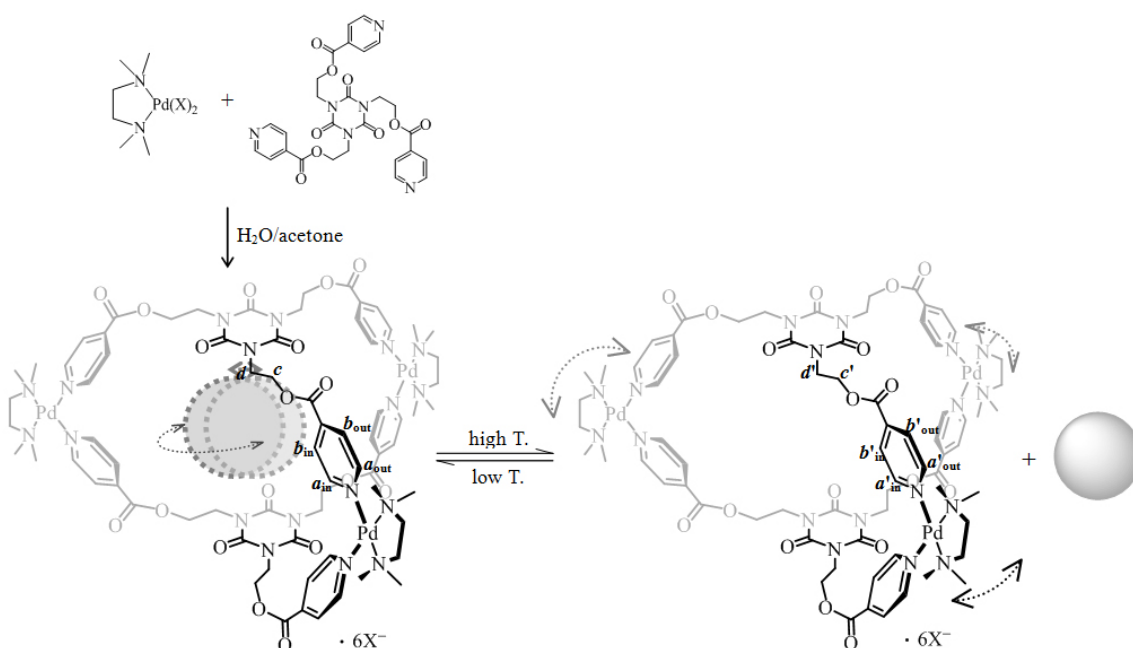
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Behavior of a Single Water Molecule within a Flexible Coordination Cage

노태환, 정옥상

부산대 화학과

In order to validate the formation and behavior of cage containing a flexible tridentate ligand, we report cage compounds, $[\text{Pd}_3\text{L}_2](\text{X})_6$ ($\text{Pd} = (\text{Me}_4\text{en})\text{Pd}(\text{II})$; $\text{X}^- = \text{BF}_4^-$ and ClO_4^-) via construction of a new C_3 -symmetric potential triangular component (L) with *cis*-protected ditopic $(\text{Me}_4\text{en})\text{Pd}(\text{II})$ as a corner linker. A single water molecule is nestled within the new cage, and is reversibly adsorbed and desorbed via a combination of the adequate space, polar environment, and conformational flexibility of the cage. Thus, the duality of liberal and restrictive properties of a single water molecule has been discussed based on spectroscopic data. In Suzuki-Miyaura C-C cross-coupling reactions, the cage complex shows significant catalytic activity along with the effects of the isolated single water molecule.



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발표분야: General Oral Presentation

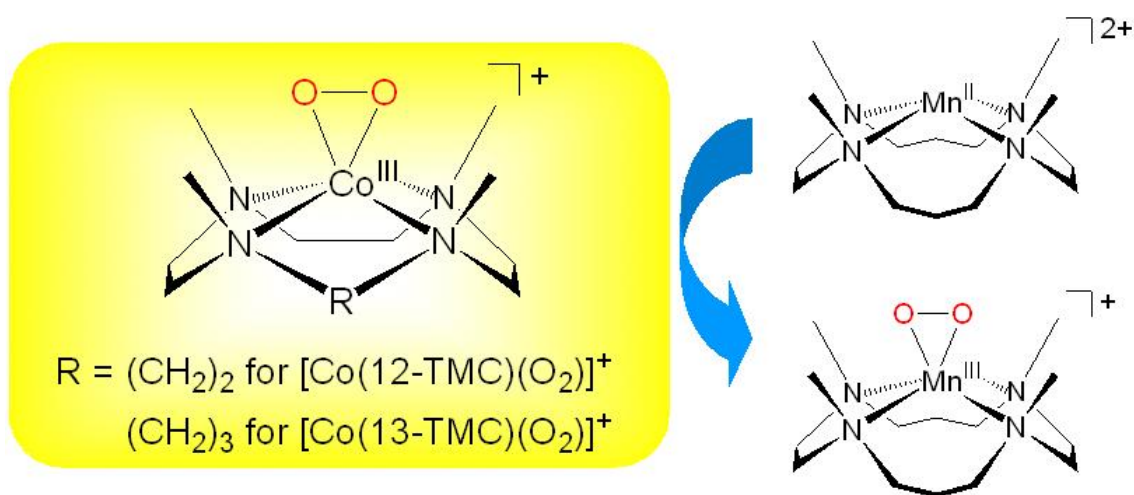
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Synthesis, Structural and Spectroscopic Characterization, and Reactivities of Mononuclear Cobalt(III)-Peroxo Complexes

강혜연, *남원우, **Edward I. Solomon

이화여대 바이오융합과학과 *이화여대 화학과 **Stanford University, USA

Metal-dioxygen adducts are key intermediates detected in the catalytic cycles of dioxygen activation by metalloenzymes and biomimetic compounds. In this study, mononuclear cobalt(III)-peroxo complexes bearing tetraazamacrocyclic ligands, $[\text{Co}(\text{12-TMC})(\text{O}_2)]^+$ and $[\text{Co}(\text{13-TMC})(\text{O}_2)]^+$, were synthesized by reacting $[\text{Co}(\text{12-TMC})(\text{CH}_3\text{CN})]^{2+}$ and $[\text{Co}(\text{13-TMC})(\text{CH}_3\text{CN})]^{2+}$, respectively, with H_2O_2 in the presence of triethylamine. The mononuclear cobalt(III)-peroxo intermediates were isolated and characterized by various spectroscopic techniques and X-ray crystallography, and the structural and spectroscopic characterization demonstrated unambiguously that the peroxo ligand is bound in a side-on η^2 fashion. The structural properties of the CoO_2 core in both complexes are nearly identical. The cobalt(III)-peroxo complexes showed reactivities in the oxidation of aldehydes and O_2 -transfer reactions. In the aldehyde oxidation reactions, the nucleophilic reactivity of the cobalt-peroxo complexes was significantly dependent on the ring size of the macrocyclic ligands, with the reactivity of $[\text{Co}(\text{13-TMC})(\text{O}_2)]^+ > [\text{Co}(\text{12-TMC})(\text{O}_2)]^+$. In the O_2 -transfer reactions, the cobalt(III)-peroxo complexes transferred the bound peroxo group to a manganese(II) complex, affording the corresponding cobalt(II) and manganese(III)-peroxo complexes. The reactivity of the cobalt-peroxo complexes in O_2 -transfer was also significantly dependent on the ring size of tetraazamacrocycles, and the reactivity order in the O_2 -transfer reactions was the same as that observed in the aldehyde oxidation reactions.



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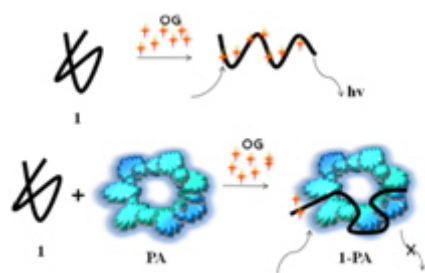
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Fluorescence Detection of Anthrax Protective Antigen with Two New DNA Aptamers

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이화여대 화학나노과학과 *이화여대 화학.나노과학과 **이화여대 화학과

Detection of PA has been found to be the most reliable assay method for the early stage of the anthracis infection, in comparison to the immunoassays directed toward LF or EF. A random single-stranded DNA (ssDNA) library was screened using the in vitro selection method (SELEX) and two DNA sequences have been developed to bind specifically to PA with high affinities at a nanomol level. The sequence of two 29-mer DNA aptamers for PA were 5'-GAT GTG GGT GTA GTT GGA GGG TAA ACG TT (1) and 5'-CAG ACC GTA AGG GAT GCC GCC TAA ACA CC. OliGreen (OG), a commercially available asymmetrical cyanine dye, has been often used to quantitate an amount of oligonucleotides. OG is weakly fluorescent in aqueous solution, but exhibits a greater enhancement in its fluorescence upon binding to single-stranded and double stranded DNA. We present a molecular fluorescence method to signal PA specifically binding the DNA aptamers using OG to label oligonucleotides noncovalently. This method for highly sensitive detection of PA using two aptamers was presented as a rapid and label-free assay. As a result of forming the DNA aptamers non-covalently bound to and surrounded by relatively big protein, the fluorescence of OG is strongly reduced. The present limit of PA detection for this system is approximately 0.1 nM. This method could be an easy and important candidate for use in bio sensing applications.



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Ligand Topology Effect on the Reactivity of High-Valent Non-heme Iron(IV)-Oxo Intermediates

홍승우, *이용민, **신운섭, ***남원우

서강대 바이오융합과 *이화여대 기초과학연구소 **서강대 화학과 ***이화여대 화학과

Understanding of the physical basis of enzymatic rate enhancement remains a critical challenge to design biomimetic novel enzymes with controlled catalytic properties. One of the most basic physical properties is the configurational orientation of the ligand system (i.e. topology). Linear tetradentate ligands can coordinate to an octahedral metal center in three different topologies, cis- α , cis- β and trans forms. In this presentation, we report the generation and reactivity comparison of iron(IV)-oxo intermediates having two different topologies of ligand. Two iron(II) complexes, $[\text{FeII}(\text{BQCN})(\text{CH}_3\text{CN})_2](\text{ClO}_4)_2$ and $[\text{FeII}(\text{BQCN})(\text{CH}_3\text{CN})_2](\text{OTf})_2$ (BQCN = N,N'-dimethyl-N,N'-bis(8-quinolyl)cyclohexanediamine), were prepared and their structures were determined by X-ray crystallography. Structural configuration of BQCN ligand in $[\text{FeII}(\text{BQCN})(\text{CH}_3\text{CN})](\text{ClO}_4)_2$ was cis- α form whereas that in $[\text{FeII}(\text{BQCN})(\text{CH}_3\text{CN})_2](\text{OTf})_2$ was cis- β form. Iron(IV)-oxo intermediates were generated by reacting two Fe(II)(BQCN) complexes with peracetic acid (3 equiv). UV-vis spectra of iron(IV)-oxo intermediates with two different topologies exhibit the characteristic peaks with different λ_{max} . We then carried out the reactivity studies of both intermediates. Interestingly, reactivity of $[\text{FeIV}(\text{O})(\text{cis-}\alpha\text{-BQCN})]^{2+}$ intermediate is ~ 10 times greater than that of $[\text{FeIV}(\text{O})(\text{cis-}\beta\text{-BQCN})]^{2+}$ intermediate in the C-H activation reaction of organic substrates.

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장소: 제주ICC

발표코드: INOR.O-14

발표분야: General Oral Presentation

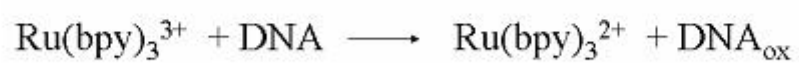
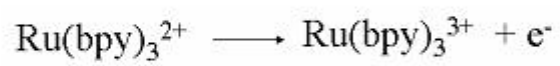
발표종류: 구두발표, 발표일시: 금 16:05, 좌장: 나명수

High Solvent Accessibility of Oligonucleotides on Small-sized Au Nanoparticles

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이화여대 나노과학부 *이화여대 화학나노과학과 **이화여대 화학과

Detection of specific oligonucleotide sequences is important for clinical diagnosis and biochemical research. Recently, the sensing methods have been developed for molecular recognition and detection, including fluorescence, SPR, AFM, quartz crystal microbalance, electrochemistry, and etc. A number of DNA-based colorimetric sensors have been reported, most of which use gold nanoparticles as sensing materials. However, most of these colorimetric methods require many steps, such as modifying and separating, which lead to complication and relatively high cost. In this presentation, we report a simple and sensitive electrochemistry sensors for DNA detection using unmodified gold nanoparticles. Single-stranded oligonucleotides containing guanine bases in their sequences were adsorbed onto gold nanoparticles (AuNPs) by a hydrophobic interaction of the bases of DNA with AuNPs. The cyclic voltammetry of $\text{Ru}(\text{bpy})_3^{2+}$ in the presence of the DNA-AuNP complex afforded an anodic current enhancement due to the oxidation of the guanine bases of DNA. (bpy=2,2'-bipyridine).



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Importance of Nanoscale SiP₂O₇ Coating on LiNi_{0.5}Co_{0.2}Mn_{0.3}O₂ Cathode Materials for High-Performance Li-ion Batteries

이용석, *조재필

울산과학기술대 친환경에너지공학부 *울산과학기술대 에너지공학부

LiNiO₂ materials have been in the spotlight as an alternative to LiCoO₂. Therefore, many methods, such as coating and doping, have been investigated to enhance the inherent problems of LiNiO₂. Naturally unstable Ni³⁺ ions are apt to reduce to Ni²⁺ on the cathode surface in the form of NiO, and further structural instability from the higher oxidation state of Ni⁴⁺ leads to substantial oxygen generation from the lattice at elevated temperatures. Particularly, the thermal instability problem leads to a faster thermal runaway than LiCoO₂. Recently, larger amounts of Ni were substituted by electrochemically inactive Mn ions (e.g., LiNi_{0.5}Co_{0.2}Mn_{0.3}O₂) to render such problems, but increasing the Mn content increased the charge transfer resistance, resulting in decreased electrochemical performance (rate capability). Moreover, half of the transition metal sites are still occupied with Ni ions. Hence, more fundamental approaches need to be investigated. In this study, we report that direct reaction of a Li source and SiP₂O₇-coated Ni_{0.5}Co_{0.2}Mn_{0.3}(OH)₂ particles leads to the simultaneous formation of an amorphous Li_xP_yO_z-like coating layer and a solid solution LiNi_{0.5-x}P_xSi_xCo_{0.2}Mn_{0.3}O₂ phase. The amorphous coating layer significantly improved the rate capability, even at 7C of rate cycling, resulting in 83 mAhg⁻¹, while the pristine cathode showed a result of 0 mAhg⁻¹. In addition, the LiNi_{0.5-2x}P_xSi_xCo_{0.2}Mn_{0.3}O₂ substantially improved by 17% the structural stability during cycling at 60°C after 40 cycles; the pristine and coated cathode show reversible capacities of 137 mAhg⁻¹ and 165 mAhg⁻¹, respectively, corresponding to 74% and 91% retention. Moreover, the evolved amount of oxygen upon an increase in the cathode at 4.5V was reduced by 1/5 compared to the pristine sample. The pristine sample shows an onset temperature of 225°C. The peak area was indicative of the total amounts of oxygen that evolved from the cathode, and this was estimated at 580 J/g. However, the coated sample showed a single peak with a greatly depressed peak height at an onset temperature of 248°C. In addition, the peak area was significantly decreased to 120 J/g.

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Single Nanorod Photovoltaic Cell Fabricated with Conducting Polymer and CdSe Blocks

유상훈, 박성호

성균관대 화학과

This contribution demonstrates a novel approach to synthesizing a bucket of nanoscale photovoltaic cells by utilizing electrochemically deposited conducting polymer and CdSe heterojunctions. Single nanorod photovoltaic cells were fabricated with the aid of electrochemical deposition and anodized aluminum oxide (AAO) templates. We successfully constructed Gold-polypyrrole-CdSe-Gold multisegment nanorods. The side metal arms simply act as a lead to facilitate their connection with microscopic circuits. This architecture showed a photovoltaic response when the white light was illuminated on the polypyrrole and CdSe domain. Excitons were separated into electrons and holes at the junction between polypyrrole and CdSe, working as a p-type and n-type semiconductor, respectively. The morphology control of each junction turned out to be critical to improving the efficiency of the resulting solar cell.

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발표종류: 구두발표, 발표일시: 금 16:20, 좌장: 나명수

Evolution of a secondary structure of LiMnPO_4 nanoparticles for a cathode material of lithium ion batteries

김태희, 송현곤

울산과학기술대 친환경에너지공학부

Encouraged by the success of LiFePO_4 (LFP), LiMnPO_4 (LMP) has attracted intensive attentions as a cathode material for lithium ion batteries. The most noticeable merit of LMP compared with LFP is based on the higher working potential of its electrochemical reaction ($\text{LiMePO}_4 \rightarrow \text{Li}^+ + \text{e}^- + \text{MePO}_4$, where $\text{Me} = \text{Mn}$ or Fe): 4.1 V versus Li^+ for LMP and 3.45 V for LFP. The higher potential enables LMP have higher energy density (= capacity x potential) even if the capacity of LMP is the same as that of LFP (170 mAh g^{-1}). However, its demerits of low electronic and ionic conductivity even poorer than those of LFP hinder the full use of the theoretical capacity of LMP. In this work, we apply our own strategy of nanostructural control to the LMP system, which successfully enhanced performances of LFP in our previous work. LMP was prepared by precipitating two intermediate precipitates sequentially. The second precipitate $\text{Mn}_3(\text{PO}_4)_2$ (MP) is obtained by adding Mn^{2+} into a solution of the first precipitate Li_3PO_4 (LP). The formation of MP is more easier than that of LP so that LP is partially solubilized with providing free phosphate ions which is consumed for making MP. The resultant structure is the hollow secondary structure consisting of spherical nanoparticles of LMP. We believe this secondary structure facilitates the access of lithium ions to LMP with smaller initial potential drop and resultantly higher capacity. In addition to the shape of LMP, homogeneous carbon coating on each primary nanoparticles was the deterministic factor for achieving good performance with LMP.

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발표분야: General Oral Presentation

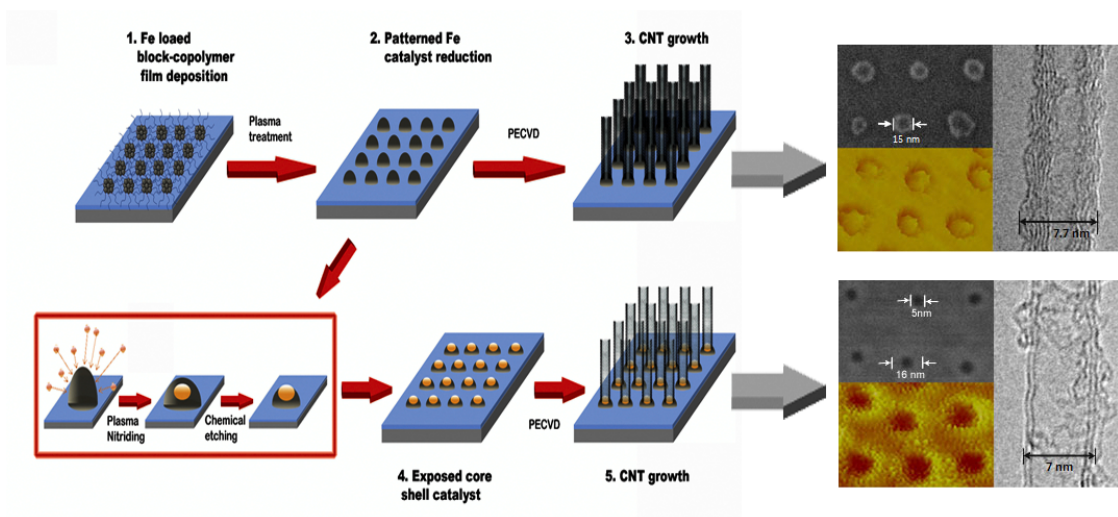
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A Facile Way to Control the Number of Walls in Carbon Nanotubes through the Synthesis of Exposed-Core/Shell Catalyst Nanoparticles

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KAIST 신소재공학과

The new exposed-core/shell (ECS) catalyst can successfully control the number of walls independently without changing the diameter of CNTs. This is because the exposed catalytically inactive core nanoparticles (iron nitride) do not involve in the growth of CNTs, while the active shell nanoparticles (iron) play as the active catalysts for growth of CNTs. The core/shell catalyst structure was shown by scanning electron microscopy (SEM), atomic force microscopy (AFM) and transmission electron microscopy (TEM), and their effect on the number of walls studied by comparison of two CNTs grown in plasma enhanced CVD from both pristine and core/shell catalysts. The number of walls in CNTs was selectively reduced to 2~3 walls in only ECS catalysts. The main two factors to control the number of walls are the confined size of the catalyst and the deactivated area of the iron nitride at the exposed core region. While the confined size of catalysts controls the diameter of CNTs, the number of inner walls in CNTs can be controlled by the inactive area composing of the iron nitride at the exposed core region of catalysts. This result implies that parameters such as the number of walls, diameters, inter-distances, and local and large area lateral distributions can be all separately adjusted if we can use core/shell catalyst nanostructures after adjusting micelle sizes and patterns.



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High-Performance Layered 3D-LiCoO₂ Cathodes with Nanoscale Co₃O₄ Coating via Chemical Etching

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울산과학기술대 친환경에너지공학부 *울산과학기술대 에너지공학부

The chemical etching of the pristine LiCoO₂ cathode material using poly(N-vinylpyrrolidone) (PVP) and silver nitrate (AgNO₃) leads morphology transition to 3D-layered by layered LiCoO₂ structure coated with nanoscale cobalt oxide layer. PVP is used for capping agent to bind with Ag⁺ ions and reduces them to Ag⁰ particles on the surface of bare LiCoO₂. The Ag coated LiCoO₂ is etched selectively to generate 3D-layered LiCoO₂ with cobalt oxide, which plays a key role of improving the electrochemical performance of LiCoO₂, as coating materials at the same time. Compared to the pristine LiCoO₂, not only 3D-layered by layered structure enhances the high rate capability (142 mAh/g at 7C), but also the nanoscale cobalt oxide coating layer improves the structure stability of LiCoO₂ at 4.6V. The etching process is expected to design other materials for the development of electrochemical performance in Li-ion batteries.

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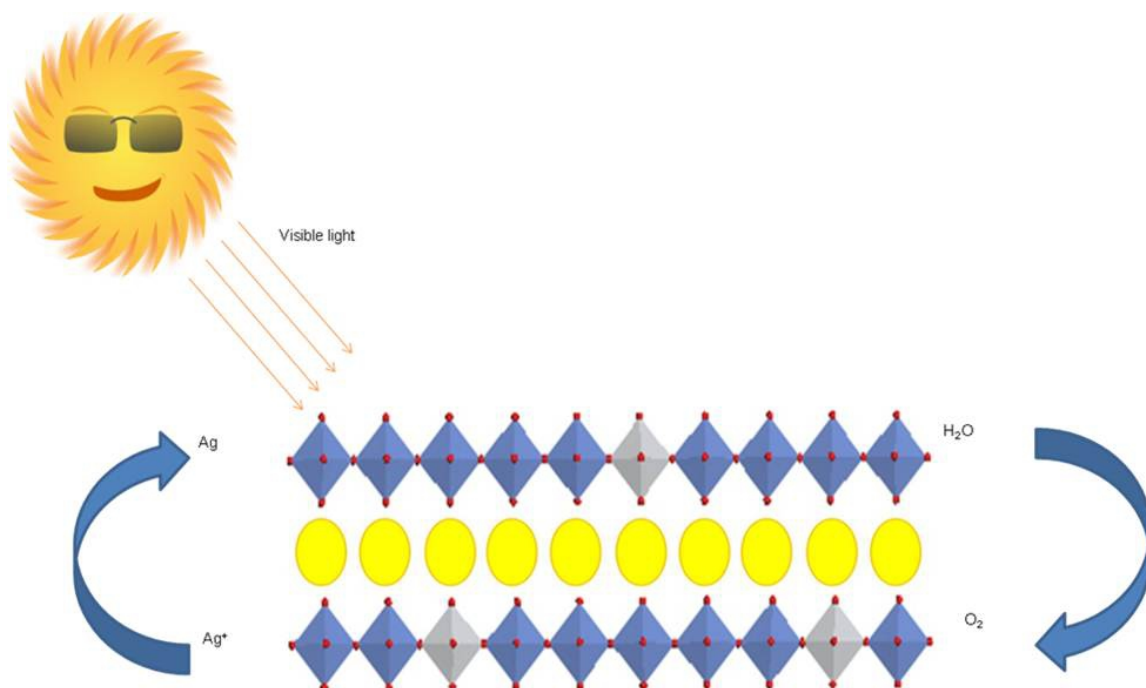
발표종류: 구두발표, 발표일시: 금 16:35, 좌장: 나명수

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

이엽, 최정훈, 최경민, 강정구

KAIST 신소재공학과

Because the current global energy consumption is primarily based on the combustion of fossil fuels that results in the pollution and the climate change on the earth, the idea of the artificial photosynthesis is considered as an appealing method to produce sustainable fuels from water and carbon dioxide. Herein, we focused on Ti embedded LDHs as candidates for water oxidation catalysts under visible light because titanium oxide is very stable under bandgap excitation. The wide band gap which is the biggest problem of titanium oxide is solved by reconstructing bandgap by introducing metal-oxygen-metal bond. We have synthesized the new titanium-embedded layered double hydroxides (LDHs) such as the (Ni/Ti)LDH and the (Cu/Ti)LDH. We find that the (Ni/Ti)LDH showed higher reaction rate of 49 $\mu\text{moles O}_2$ for water oxidation by using 200 mg of the photocatalyst and 1 mmol of AgNO_3 as a sacrificial agent. Also, the (Cu/Ti)LDH showed a good reaction rate of 31 μmoles under the same condition. Moreover, we have determined what part of the visible light is actually responsible for the oxygen generation so that the source light for metal to metal charge transfer of the LDH photocatalysts are figured out as blue light.



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Thermal and electrochemical stability of the MnO₂coated Li[Ni_{0.7}Co_{0.15}Mn_{0.15}]O₂ cathode material

조용현, *조재필

울산과학기술대 친환경에너지공학부 *울산과학기술대 에너지공학부

In an attempt to overcome the problems associated with LiNiO₂, the solid solution series of lithium nickel-metal oxides, Li[Ni_{1-x}M_x]O₂ (with M = Co, Mn, Al, Ti, Mg, etc.), have been investigated as favorable cathode materials for high-energy and high-power lithium-ion batteries. However, upon heating to 300°C, the delithiated cathodes undergo a faster phase transformation into the NiO-type rock salt phase with releasing oxygen, leading to thermal runaway of the cell. Here, we report a MnO₂ coated Li[Ni_{0.7}Co_{0.15}Mn_{0.15}]O₂ cathode material which has a high energy and safety. The material demonstrates reversible capacity of 200 mAhg⁻¹ and retains 95% capacity retention at the most severe test condition of 60°C. In addition, amount of oxygen evolution from the lattice in the MnO₂ coated cathode is reduced by 70%, compared to the reference sample. All these results suggest of MnO₂ coated Li[Ni_{0.7}Co_{0.15}Mn_{0.15}]O₂ satisfy the requirements for hybrid electric vehicles, power tools, and mobile electronics.

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Investigation of the formation mechanism and the magnetic properties of magnetic multi-granule nanocluster

차진명, 이진규

서울대 화학부

The development of magnetic nanocrystals with high magnetic response is of great importance for several applications. Recently, the convenient synthesis of magnetic multi-granule nanoclusters (MMGNs) was reported by the reaction of FeCl_3 in ethylene glycol as solvent as well as reductant in the presence of sodium acetate. However, the precise formation mechanism of nanoclusters is not clear. We have systematically studied the formation of MMGNs to suggest the mechanism involving the following steps: 1) hydrolysis/condensation of FeCl_3 in the presence of NaOAc , 2) phase transition from amorphous ferrihydrite to crystalline iron oxide hydrate, and 3) partial reduction Fe^{3+} to Fe^{2+} by ethylene glycol and 2nd phase transition (iron oxide hydrate \rightarrow magnetite) via multi-sites nucleation and growth to nanoclusters within iron oxide hydrate crystals. Based on the mechanism, the size of MMGNCs can be precisely controlled from about 30 nm to about 800 nm by varying initial reaction conditions. By refluxing at atmospheric pressure, unlike the conventional autoclave method, it is possible to conduct a large-scale synthesis up to few tenth gram-scales. The magnetic saturation values of the MMGNs are close to that of bulk magnetite materials, and the MMGNs showed hysteresis loops in the M-H curves at RT, indicating the ferrimagnetic nature of the MMGNs. More detailed results of the investigation of synthetic mechanism and magnetic properties of the MMGNs will be discussed.

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발표종류: 구두발표, 발표일시: 금 16:50, 좌장: 나명수

A facile chemical route of various metal oxides synthesis and their application as an efficient photocatalysts

Nitin Chaudhari, *유종성

고려대 소재화학과 *고려대 신소재화학과

The architectural controlled synthesis of nanostructure semiconductors has received much research attention, due to their outstanding physical and chemical properties and potential applications in numerous fields. Obtaining new materials via a relative simple route and developing the morphology-controlled synthesis methodologies are a goal and evoke great interest in materials chemistry. In recent years, considerable attention has been given to the environmental problem involving organic pollutants in water. Photocatalysis is a promising technology for the treatment of contaminants, especially for the removal of organic compounds and also for the water splitting. Many investigations have been reported on utilizing metal oxide nanomaterials as photocatalysts to decompose or destroy the organic pollutants in water. In this work, we synthesized various hierarchical metal oxides, iron oxide, zinc oxide, nickel oxide, cobalt oxide, manganese oxide, etc by a newly designed hydrothermal self-assembly process. The photocatalytic activity of these architectures has been tested by the degradation of Rhodamine B (RhB) under UV and Visible light irradiation, showing that the as-prepared metal oxide structures exhibit high photocatalytic activity for the degradation of RhB.

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장소: 제주ICC

발표코드: INOR.O-24

발표분야: General Oral Presentation

발표종류: 구두발표, 발표일시: 금 16:55, 좌장: 나명수

Fabrication of size controlled cobalt nanoparticles on carbon nitride nanotubes using sodium hypophosphite and their application as a catalyst for hydrogen generation

송철욱, *최화섭, 강정구

KAIST 신소재공학과 *KAIST EEWS

We reported a facile route to fabricate size-controlled cobalt nanoparticles (Co NPs) on carbon nitride nanotubes (CNNTs) including heterogeneous nitrogen in the Carbon nanotubes. The size of the Co nanoparticles was controlled down to 2 nm. This fabrication method was based on the reduction of cobalt ions via the mediation of two H-adatoms bonded on the pyridine-like nitrogen of the CNNTs using microwave radiation in the presence of sodium hypophosphite (Na^+ , H_2PO_2^-), water, cobalt precursor (Co^{2+} ions) and OH^- ions. We applied the fabricated Co NPs-CNNTs hybrids to the catalytic activities for hydrogen generation in an alkaline sodium borohydride (NaBH_4) aqueous solution with high-capacity hydrogen storage, and got the high hydrogen generation rate of 19.6 kg/h per kg of catalyst. This superior catalytic activity (about 82 times higher than that for the Co powder in the bulk state) is attributed to the increase of surface area reacting with solution by the size-controlled Co NPs catalysts formed via mediation of the two H-adatoms bonded to the pyridine-like nitrogen.

일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: **PHYS.O-1**

발표분야: Recent Trends in Physical Chemistry

발표종류: 구두발표, 발표일시: 금 13:00, 좌장: 이영민

Adsorption Structure of Amino Acids on Ge(100) Surface: Competition among Functional Groups

이한길

숙명여대 화학과

Functionalization of biomolecules such as amino acids is a growing field of fusion technologies that has recently emerged. The manipulation of interactions between biological and inorganic systems at the molecular level would assist a fundamental understanding of interfacial phenomena for potential applications in nanobiotechnology and biomedical sciences through biological interactions. Organic materials may be easily tailored to tune their properties via substitution and addition reactions, so that organic functionalization may be readily exploited in applications such as biosensors, biochips, and electronic devices. Recently, several studies have examined the adsorption of amino acids on surfaces. Our group has studied the adsorption structures and behavior of amino acids specifically on Ge(100) to lay the groundwork for fabricating new bio-electronic hybrid devices. Here we will demonstrate the adsorption structure for various amino acids adsorbed on Ge(100) surface such as phenylalanine, tyrosine and serine. The adsorption configurations of amino acids adsorbed on a Ge(100) surface have been studied using core-level photoemission spectroscopy (CLPES) and Density Functional Calculation (DFT) to scrutinize the adsorption structure as a function of coverage. Analysis of the C 1s, N 1s, and O 1s core-level spectra revealed quite different structures depending on the methionine coverage. We found that at low coverage (~ 0.30 ML), an O-H dissociated-N dative bonding structure is favorable. On the other hand, O-H dissociated bonding configuration was observed at a higher coverage (0.60 ML and above). We will explain precisely the results using CLPES and DFT calculations.

일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: **PHYS.O-2**

발표분야: Recent Trends in Physical Chemistry

발표종류: 구두발표, 발표일시: 금 13:20, 좌장: 이영민

Ultrafast Chemical Exchange in Condensed Phase studied by 2D-IR

곽경원, *Daniel Rosenfeld, *Michael D. Fayer

중앙대 화학과 *Stanford University Chemistry Department

A wide variety of molecular systems undergo fast structural changes under thermal equilibrium conditions. Although the rate of an overall process may be slow, key events on the molecular level are fast. Measuring these fast equilibrium dynamics without changing equilibrium behavior is at the forefront of chemical research. With the recently developed ultrafast 2D-IR spectroscopy, I can measure the formation and dissociation rate of weak hydrogen bonding complexes, the rate of rotational gauche-trans isomerization around carbon-carbon single bond, and the structural transformation of a protein within picosecond time scale. In addition to these two-state exchanges, recently more complex reactions including three-state are studied with Sn-1 type hydrogen bonding partner exchange and hydrogen bond migration within one molecule. Especially hydrogen bonding partner exchange reaction is more closely related to the Sn-1 type substitution reaction which includes bond breaking, diffusion and new bond forming. Also hydrogen bond migration study shows one example to differentiate one kinetic pathway from others. In this talk, the basic features of 2D-IR spectroscopy and how to extract the exchange rate from the spectrum for each reaction step of three state exchange reaction.

일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: **PHYS.O-3**

발표분야: Recent Trends in Physical Chemistry

발표종류: 구두발표, 발표일시: 금 13:40, 좌장: 이영민

Distance dependences of charge transfer mechanisms

김희영, 심은지

연세대 화학과

Long-range charge transfer (CT) processes in Donor-Bridge-Acceptor (DBA) system are of current interest because of their relevance to the development of molecular electronics. Long-range CT is known to occur via two fundamentally different mechanisms, a single-step tunneling process and a multistep charge-hopping process, depending on the distance decay constant (β) which describes the steepness of the exponential decrease of CT rates with increasing donor-acceptor distance. In the general theory of bridge-mediated CT processes, existence of intermediate regime between the tunneling and the hopping regime have been ignored. Recently, the intermediate regime has been discussed in several reports. We have found various complex mechanisms as well as intermediate regime depending on the distance decay constant. In addition to rate estimating based on density matrix computation, density matrix decomposition based on the path integral formalism provides relative contribution of possible charge transfer mechanisms such as incoherent (nearest-neighbor) hopping, through-bridge, and superexchange mechanism. The distance decay constant is a sensitive function of the entire DBA combination. We present a quantitative relationship between the experimentally determined distance decay constant and the magnitude of the tunneling energy gap.

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장소: 제주ICC

발표코드: **PHYS.O-4**

발표분야: Recent Trends in Physical Chemistry

발표종류: 구두발표, 발표일시: 금 13:50, 좌장: 이영민

The entropy–hydrogen bond molecular dance: thermodynamics of water confined in nanotubes

Tod A. Pascal, *William A. Goddard III

*KAIST EEWS *California Institute of Technology*

Water is a very special liquid that involves the interplay of hydrogen (H) bonding, dipole and entropic interactions, giving rise to its function and several unique properties such as the wetting and complete filling of carbon nanotubes (cnts). Here we report the thermodynamic origin of the favorable confinement of water in cnts using extensive molecular dynamics simulations and explicit calculation of entropy. We find that water molecules confined in the armchair cnts of all sizes have a lower chemical potential as compared to the bulk, resulting from decreased enthalpy in the (8,8) and (9,9) tubes and increased entropy for all other nanotubes, counter-intuitive to a textbook picture that confinement generally leads to a decrease in entropy and, when creating a surface, would necessarily break water-water H-bonds with an enthalpic penalty. We find a thermodynamic transition from a low-density vapor-like phase of water for small cnts [(6,6) and (7,7)], to an ice-like phase for medium sized cnts [(8,8) and (9,9)], then to a bulk-like liquid phase for larger tubes [beyond (12,12)]. Simulations with structureless coarse grained water models further reveal that the favorable free energies of water under confinement and the latter transition arise from the tetrahedral structural nature of liquid water. The results provided here offer a broad theoretical basis for understanding water transport through cnts that is critical in the field of nano-fluidics and filtrations.

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장소: 제주ICC

발표코드: **PHYS.O-5**

발표분야: Recent Trends in Physical Chemistry

발표종류: 구두발표, 발표일시: 금 14:10, 좌장: 성봉준

Actuation of self-assembled two-component rod-like nanostructures

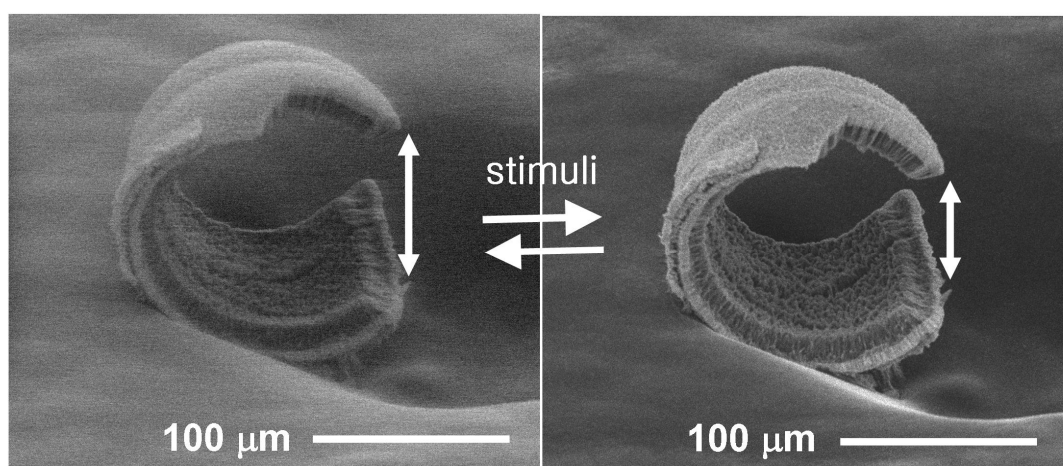
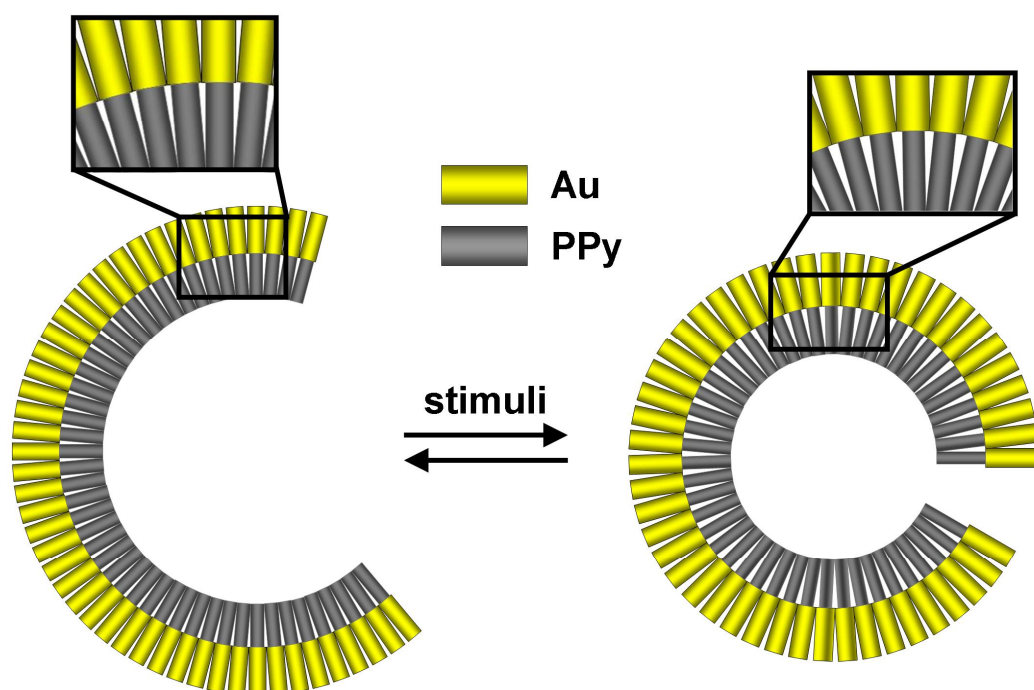
임종국, *Jacob W. Ciszek, **Fengwei Huo, ***Jae-Won Jang, ****Chad A. Mirkin

조선대 화학과 *Department of Chemistry, Loyola University Chicago, USA **School of Materials

Science and Engineering, Nanyang Technological University, Singapore ***NanoInk Inc., USA

****Department of Chemistry, Northwestern University, USA

A model for predicting the effects of stimuli-induced contraction of the polypyrrole ends of two-segment gold-polypyrrole nanorods on their assembly into curved superstructures is presented. The model and experimental data presented here show that small changes (ca. 3%) in the diameter of the polypyrrole segment of each rod will induce dramatic changes (up to 20%) in the radii of the resulting superstructures, providing a convenient means for actuating their opening and closing. We show experimentally that this actuation can be affected via humidity, temperature, and light.



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장소: 제주ICC

발표코드: **PHYS.O-6**

발표분야: Recent Trends in Physical Chemistry

발표종류: 구두발표, 발표일시: 금 14:30, 좌장: 성봉준

Quantitative and isotopic analysis of nuclear materials in swipe and environmental samples using thermal ionization mass spectrometry

박종호, 송규석

한국원자력연구원 원자력화학연구부

Highly accurate and precise analysis of nuclear materials in swipe and environmental samples plays important roles in monitoring undeclared nuclear activities for safeguards and nuclear forensics. As the samples contains ultra-trace amounts of nuclear materials, the analysis requires advanced chemical treatments and highly sensitive measurement techniques. Conditions of a series of sample treatment techniques consisting of sample ashing and acid digestion were optimized for high recovery yield. UTEVA was utilized for complete chemical separation of uranium and plutonium contained in samples. The recovery yield after chemical separation was determined as over 90% using MC-ICP-MS measurements. Highly precise thermal ionization mass spectrometry (TIMS) with isotope dilution mass spectrometry (IDMS) technique were employed for quantitative and isotopic measurements with developments in background minimization and data correction for enhanced accuracy. The current analytical techniques and procedures managed with a QA/QC system satisfying ISO/IEC 17025 was verified with analysis using certified reference materials showing excellent agreements with the certified values

일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: **PHYS.O-7**

발표분야: Recent Trends in Physical Chemistry

발표종류: 구두발표, 발표일시: 금 14:50, 좌장: 성봉준

Spatial separation of structural isomers and hydrogen bonded complex by molecular deflector

안두식, 김상규

KAIST 화학과

The separation of molecules is important as the first step of investigations of structure related chemical and physical properties. A clear spatial separation of cis- and trans-isomer of 3-aminophenol is accomplished with the electrostatic molecular deflector and velocity modulation of molecular beam. The hydrogen bonded complex with one water molecule is also separated and characterized with REMPI spectroscopy. The simulation reproduces the observed deflection profiles well.

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장소: 제주ICC

발표코드: **PHYS.O-8**

발표분야: Recent Trends in Physical Chemistry

발표종류: 구두발표, 발표일시: 금 15:00, 좌장: 성봉준

Development for Supported Membrane Biosensor

김용훈

농촌진흥청 농업공학부

Supported membrane is commonly used as a model membrane for in vitro study and biotechnological application, such as biochip and biosensors for medical diagnosis and screening for discoveries of new drug. The effect of the electrostatic attractive force between giant unilamellar vesicle (GUV) and the SiO₂ surface on the formation of Ca²⁺ free supported lipid bilayer (SLB) was investigated by atomic force microscopy and fluorescence microscopy. When negatively charged GUV were incubated for 1h without Ca²⁺, the surface coverage of lipid bilayer was < 1% on the SiO₂ surface, In contrast, a high coverage was obtained without addition of Ca²⁺ on positively charged surface modified by aminopropyltrimethoxysilane (APS), and the coverage of SLBs decreased with increasing KCl concentration. The thickness of water layer under SLBs was reduced by modification of APS. On a specially fabricated microelectrode by the surface of SiO₂ (600 nm)/CoSi₂ (10 nm)/Si substrate, a lipid bilayer was formed by employing GUVs fusion and electrical property of SLB electrode was measured.

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장소: 제주ICC

발표코드: **PHYS.O-9**

발표분야: Recent Trends in Physical Chemistry

발표종류: 구두발표, 발표일시: 금 15:20, 좌장: 김희영

Energetics and Quantum Conductance of Ferrocene-adsorbed Graphene and Graphene Nanoribbon under heteroatom doping.

강홍석, *Anup Pramanik

전주대 나노신소재공학과 *전주대 공학연구소

Based on the PBE-D2 calculation that empirically includes van der Waals interaction to the standard GGA approximation of Perdew, Berke, and Ernzerhof (PBE), we have investigated the adsorption of ferrocene molecule on the pristine, B-doped, and N-doped graphene and graphene nanoribbon. First, we find that the heteroatom dopings increase the binding energy of ferrocene. Second, our calculation of the quantum conductance using nonequilibrium Green's function method in combination with the PBE DFT indicates that those dopings do not break the ballistic transport at the Fermi level. Furthermore, we also find that the B-doping introduces an extra eigenchannel through which electron can transport at low biases.

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장소: 제주ICC

발표코드: **PHYS.O-10**

발표분야: Recent Trends in Physical Chemistry

발표종류: 구두발표, 발표일시: 금 15:30, 좌장: 김희영

Charge doping in graphene on highly polar mica

심지혜, 고택영, 류순민

경희대 응용화학과

Graphene, one single atomic layer of graphite, has attracted extensive attention in various research fields since its first isolation from graphite. Application in the future electronics requires better understanding and manipulation of electronic properties of graphene supported on various solid substrates. Here, we present a study on charge doping and morphology of graphene prepared on atomically flat and highly polar mica substrates. Ultra-flat single-layer graphene was prepared by micro-exfoliation of graphite followed by deposition on cleaved mica substrates. Atomic force microscopy (AFM) revealed presence of ultra-thin water films formed in a layer-by-layer manner between graphene and mica substrates. Raman spectroscopy showed that a few angstrom-thick water films efficiently block electron transfer from graphene to mica. Hole doping in graphene caused by underlying mica substrates was also visualized by scanning Kelvin probe microscopy (SKPM).

일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: **PHYS.O-11**

발표분야: Recent Trends in Physical Chemistry

발표종류: 구두발표, 발표일시: 금 15:40, 좌장: 김희영

Graphene nanohybrid film fabrication and study on the optical properties

Monica Samal, 이동기, *이창렬

경원대 바이오나노학부 *광주과학기술원 고등광기술연구소

The device performance of organic solar cell using multilayer graphene on amorphous PET (PETG) substrate as the electrode is studied. The change in surface morphology of the PETG substrate upon thermal annealing are investigated by atomic force microscopy (AFM), field emission scanning electron microscope (FE-SEM) and current-voltage characteristics. When thermally annealed, the graphene surface becomes rougher and more wrinkled in nanometer scale size, compared to the decrease in roughness of graphene surface in micrometer scale size. The openings created by the bubbles in the graphene layer were filled by the thermal expansion of PET substrate. However, the initial cracks originated on the graphene by the surface stress between the graphene and PET layer grew up and deteriorated the device performance. The PETG device showed the poor performance compared to ITO glass as the electrode. To summarize, the device performance using PETG substrate is strongly related to graphene surface morphology.

일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: **PHYS.O-12**

발표분야: Recent Trends in Physical Chemistry

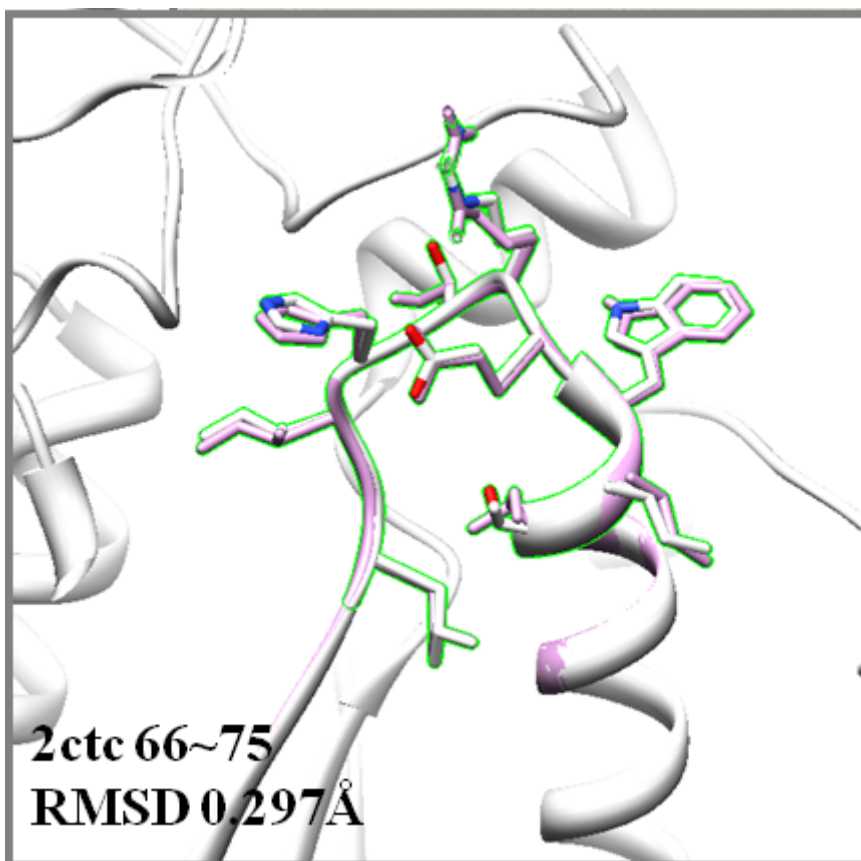
발표종류: 구두발표, 발표일시: 금 15:50, 좌장: 김희영

Protein Loop Modeling and its Applications

박한범, 석차욱

서울대 화학부

Protein loops are often responsible for functional specificity of a given protein by contributing to recognition of interaction partners, enzymatic reactions with substrates, or conformational changes relevant to function. The special properties of protein loops originate from the variable loop structures that occur as a result of substitutions, insertions or deletions in sequence during evolution. In this presentation, a novel method for structure prediction of such variable regions is described. The method is based on the analytic loop closure algorithm that can efficiently sample geometrically consistent loop structures. An energy function based on physicochemical properties and statistical preferences of amino acids guides loop models to more accurate conformations. This method was applied to the 9th Critical Assessment of techniques for protein Structure Prediction (CASP9), a bi-annual world-wide protein structure prediction experiment. The loop modeling method made significant contributions to the performance of our structure prediction method which was recognized as one of the top-ranking methods in CASP9. It is also demonstrated that this study has a great potential for applications to challenging biophysical problems that involve protein loops.



일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: **PHYS.O-13**

발표분야: Recent Trends in Physical Chemistry

발표종류: 구두발표, 발표일시: 금 16:00, 좌장: 김희영

Host-Guest Chemistry in Gas Phase: Selected Fragmentations of CB[6]-peptide Complexes at Lysine Residue

허성우, 박경만, 김승빈, 김기문, 김준곤

포항공과대 화학과

Cucurbit[n]uril (CB[n], $n = 5-10$) is neutral cyclic molecule, which comprises n glycoluril [$=C_4H_2N_4O_2=$] repeat units. Each glycoluril unit is joined to the next one by two methylene [$-CH_2-$] bridges to form a closed band. CB[n] are efficient host molecules in molecular recognition and have high affinity for positively charged or cationic compounds. Their host-guest properties allow various applications of these molecules including drug deliveries, reaction catalysts, etc. In this study, we investigate the host-guest property of CB[6] to lysine residues in gas phase along with peptide dissociations related to mobile proton model by electrospray ionization mass spectrometry (ESI-MS) and electrospray ionization tandem mass spectrometry (ESI-MS/MS) in the positive ion mode. All model peptide complexes exhibit a common highly selective product at m/z 549, which corresponds to the CB[6] complex of 5-iminopentan-1-aminium in collision induced dissociation tandem mass spectrometry (CID-MS/MS) spectrum. The energy required for proton mobilization from N-terminus to lysine amide backbone strongly depends on location of the residue. The overall reaction to yield CB[6] complex of 5-iminopentan-1-aminium product exothermic due to the strong host-guest interaction between 5-iminopentan-1-aminium and CB[6].

일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: **PHYS.O-14**

발표분야: Recent Trends in Physical Chemistry

발표종류: 구두발표, 발표일시: 금 16:10, 좌장: 김희영

The excited state simulations of firefly bioluminescence system

송창익, 이영민

포항공과대 화학과

We have tried various theoretical approaches to reveal the nature of firefly bioluminescence. Firstly, we build the system consisting of the chromophore oxyluciferin, the enzyme luciferase, and the solvating water molecules to mimic the actual physiological emitting condition. Because the excited state surface information is essential when dealing with luminescence, the excited state parameters were constructed with our newly developed methods of the argon-scanning and Hessian-matching. Then, we have performed molecular dynamics (MD) simulations of the system on both the ground and the excited states. We find that the aspects on the two surfaces show distinctive characteristics in terms of solvating water structure around oxyluciferin. In addition, we have studied the emission mechanism from these MD ensembles with the help of quantum-mechanics/molecular-mechanics (QM/MM) approach to address the relationship between the color variation and the solvation dynamics. Finally, we remark the importance of considering luminescing time scale for such analysis.

일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: **PHYS.O-15**

발표분야: Recent Trends in Physical Chemistry

발표종류: 구두발표, 발표일시: 금 16:20, 좌장: 김희영

PAG Bound PMMA-Based Resist polymers

손경화, *김민정, **이해원

한양대 나노과학기술연구소 *한양대 화학과 **한양대 화학과, 나노과학기술연구소

PMMA-based electron beam resists have been widely used for mask fabrication. Recently, PAG grafting into the main chain of the polymer resists was reported. Advantages of PAG-bound polymer resists are PAG outgassing, higher loading of PAG without aggregation or phase separation, and uniform distribution of PAG. Our group has reported the novel photoacid-generating methacrylate monomer with a triphenylsulfonium triflate moiety as the PAG was prepared and co-, terpolymerized with other monomers to obtain the PAG bound polymer resist materials. We have applied E-beam, AFM, ArF and KrF excimer laser lithography in order to demonstrate the effect of the polymer bounded PAG resists. These resists were successfully applied for fabrication of nano-scale patterns.

일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: **PHYS.O-16**

발표분야: Recent Trends in Physical Chemistry

발표종류: 구두발표, 발표일시: 금 16:30, 좌장: 김희영

Hollow Core-Mesoporous Shell Carbon Sphere for High Li Storage Capacity and Better Cycling

김민식

고려대 신소재화학과

Hollow Core-Mesoporous Shell Carbon spheres (HCMSC) with hierarchical nanostructure was prepared and explored as anode in Li ion battery. Compared with commercial graphite and Ordered Mesoporous Carbon (CMK-3), the HCMSC not only demonstrates higher Li storage capacity, but also better cycling performance and rate capability. HCMSC possesses unique structural characteristics such as large surface area and mesopore volume, particularly the multimodal porosity composed of well-developed 3D interconnected mesopores embedded in the mesopore shells, facilitating fast mass transport and charge transfer. The enhancement in anode performance especially in the cycling performance and rate capability is mainly attributable to the superb structural characteristics of the HCMSC. These includes particularly the macropore of core encapsulated in well-developed 3D interconnected mesoporous shell, possibly act as efficient Li storage and buffer reservoirs to reduce volume change during the charge-discharge cycling especially at high rates.

일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: ORGN.O-1

발표분야: Oral Presentation for Young Organic Chemists

발표종류: 구두발표, 발표일시: 금 09:30, 좌장: 강은주

Synthesis and Characterization of Cross-linked and Reinforced composite membrane Using Cyclodimerization of Trifluorovinyl Ether Groups for Fuel Cell Applications

이혜진, *김병각, **김형준

서울대 화학생명공학부 *한국화학연구원 정보전자폴리머연구센터 **KIST 연료전지센터

PEFCs (polymer electrolyte fuel cells) have attracted as one of alternative and environmentally friendly energy sources for portable and stationary applications. Perfluorosulfonated polymer such as Nafion is widely used as the PEM (proton-exchange membrane) due to its high proton conductivity and good chemical and mechanical properties. However, Perfluorosulfonated polymer membranes suffer from high cost and low conductivity at high temperature. As an effort to overcome these drawbacks, studies have been conducted on hydrocarbon-based polymer electrolyte membrane such as sulfonated poly(ether sulfone)s and sulfonated poly(arylene ether)s. Much progress on hydrocarbon-based polymer membranes has been made, while we still have difficulties in making a balance between hydrophilic character for high proton conductivity and hydrophobic nature required to obtain physical stability. In this study, we present synthesis and characterization of cross-linked and reinforced composite membrane using cyclodimerization of trifluorovinyl ether groups for fuel cell applications. The highly sulfonated PES shows good proton conductivity but low mechanical properties. The one of effective ways to make highly sulfonated PES having good physical properties is cross-linking. The trifluorovinyl group can be cross-linked at relatively low temperature (>120 °C), does not require catalyst, and does not produce by-product. For this reason, trifluorovinyl group was introduced at the end of fully sulfonated PES and pasted onto reinforced membrane. After thermal treatment, the composited membrane showed high dimensional stability and proton conductivity compared to Nafion212.

일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: ORGN.O-2

발표분야: Oral Presentation for Young Organic Chemists

발표종류: 구두발표, 발표일시: 금 09:40, 좌장: 강은주

Acetylene Gas Mediated Conjugated Microporous Polymers (ACMPs): First Use of Acetylene Gas as a Building Unit

최정훈, 최경민, 이엽, 강정구

KAIST 신소재공학과

Here, we report the new microporous nanostructures so called "Acetylene Gas Mediated Conjugated Microporous Polymers (ACMPs)" using acetylene gas as a building unit with functional linkers via the coupling reaction, where the acetylene gas was used as a source of the functional building unit for the first time. Three types of ACMPs have been synthesized in this work. ACMP-C was fabricated by linking Tetrakis(4-iodophenyl) methane with an acetylene gas, whereas ACMP-C6 and ACMP-N were synthesized from 1,3,5-Tris(4-iodophenyl) benzene and Tris(4-iodophenyl) amine, respectively. The structures with the triple-bond linkages have been confirmed by the solid-state ^{13}C CP MAS NMR, consistent with those obtained from FT-IR measurements. Additionally, it is considered that our new approach will be on a great breakthrough to synthesis of the microporous nanostructures linked with functional organic building units enabling the advanced modification after synthesis, like organo-metallic complexes decoration or metal cation-doped porous nanostructures where metal cation could be anchored on the organic linkers.

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장소: 제주ICC

발표코드: ORGN.O-3

발표분야: Oral Presentation for Young Organic Chemists

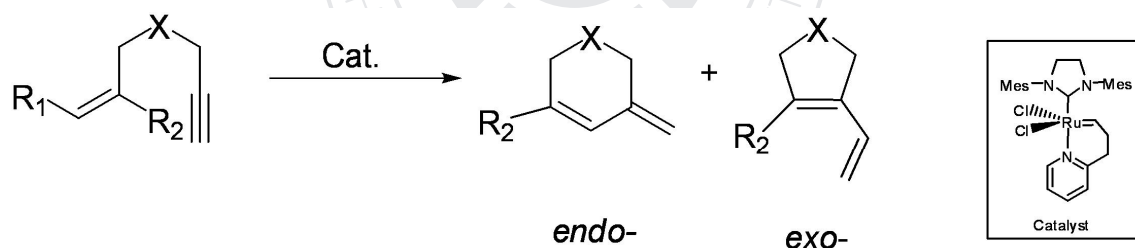
발표종류: 구두발표, 발표일시: 금 09:50, 좌장: 강은주

Studies on Ring-closing Enyne Metathesis of Various Methyl Substituted Substrates

송정아, 나영임, 한소엽

이화여대 화학나노과학과, 촉매반응·합성연구센터

Ring-closing enyne metathesis (RCEYM) with heteroatom (N, O)-containing enyne substrates has been studied by using pyridine-chelating ruthenium catalyst. Location of the methyl substituent of the enyne moiety played the major role in determining the regiosomeric product ratio. The detailed results will be discussed at the presentation. This work is supported by the NRF (WCU project R33-10169).



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발표코드: ORGN.O-4

발표분야: Oral Presentation for Young Organic Chemists

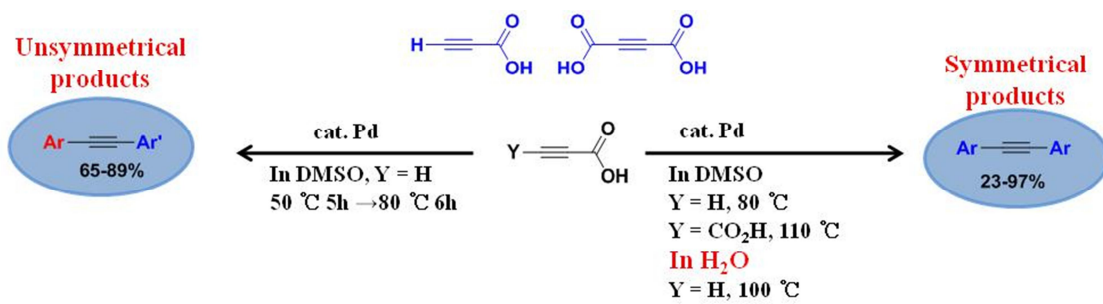
발표종류: 구두발표, 발표일시: 금 10:00, 좌장: 강은주

Diarylalkynes synthesis by palladium catalyzed decarboxylative Sonogashira reaction

박경호, 이선우, Thiruvengadam Palani

전남대 화학과

Symmetrical diarylalkynes were obtained from the decarboxylative coupling reactions of arylbromides and propiolic acid (or 2-butyndioic acid) in good yields. The optimized reaction conditions were 2.0 equiv. of arylbromide, 1.0 equiv. of propiolic acid (or 2-butyndioic acid), 5.0 mol% Pd(PPh₃)₂Cl₂, 10.0 mol% 1,4-bis(diphenylphosphino)butane(dppb), 2.0 equiv. of 1,8-diazabicyclo[5.4.0]undec-7-ene(DBU), and dimethylsulfoxide(DMSO) or Water(H₂O) as the solvent. The coupling reaction of propiolic acid with arylbromides required 80 °C but the reaction of 2-butyndioic acid with arylbromides required 110 °C. Interestingly, When water used for the solvent also symmetrical diarylalkynes were obtained from the decarboxylative coupling reactions of arylbromides and propiolic acid in good yields. In the presence of phase transfer surfactant C₁₈H₃₇N(CH₃)₃Cl, the catalytic system of both Pd(PPh₃)₂Cl₂/dppb and Pd(TPPMS)₂Cl₂/TPPMS afforded the desired coupled products in good yields. In the coupling reaction of propiolic acid with arylbromides, the diarylated product was the major one at 80 °C, even though 1 equiv. of arylbromide was employed. However, among the mono arylated products that were formed predominantly at 25 and 50 °C in the coupling reaction with aryl iodide, more Sonogashira coupling product was obtained than the decarboxylative coupling product. Unsymmetrical diarylalkynes were also synthesized via this method, in which all reagents, including propiolic acid, aryl iodide, and arylbromides were added at the beginning of the reaction.



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발표코드: ORGN.O-5

발표분야: Oral Presentation for Young Organic Chemists

발표종류: 구두발표, 발표일시: 금 10:10, 좌장: 강은주

An Efficient Synthesis of Phthalides and Isocoumarins in *N*-Heterocyclic Carbene Catalysis

박종협, 윤소원

한양대 화학과

In recent years, *N*-heterocyclic carbenes (NHCs) emerged as a promising organocatalyst for the development of new synthetic methodologies in organic synthesis due to their unique reactivities. Here, we report an efficient NHC-catalyzed synthesis of phthalides and isocoumarins from 2-alkynylbenzaldehydes under aerobic conditions. Depending on the nature of substituents at the alkyne terminus, phthalides and isocoumarins could be formed selectively via either 5-*exo-dig* or 6-*endo-dig* pathway, respectively.

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장소: 제주ICC

발표코드: ORGN.O-6

발표분야: Oral Presentation for Young Organic Chemists

발표종류: 구두발표, 발표일시: 금 10:20, 좌장: 강은주

Orthogonal Regioselective Synthesis of N-alkyl-3-substituted Tetrahydroindazolones

김종훈, *박승범

서울대 화학과 *서울대 화학부

SNX-2112, which contains a tetrahydroindazolone moiety, has been identified as a potent heat shock protein 90 (HSP90) inhibitor and exhibits low nanomolar antiproliferative activities against multiple cancer cell lines. In spite of their proven importance in biomedical research, the regioselective synthesis of N-alkyl-3-substituted tetrahydro-indazolones has not been studied extensively as compared with N-aryl-3-substituted tetrahydroindazolones. As reported in the literature, a major strategy for the orthogonal regioselective synthesis of N-aryl-tetrahydroindazolone involves the condensation of appropriate dielectrophiles such as 2-acylcyclohexane-1,3-dione or enol ether derivatives of 2-acylcyclohexane-1,3-dione with an arylhydrazine. However, this method cannot be extended to alkylhydrazines because of the similar nucleophilicities of two amines, which lead to yield the regioisomeric mixtures of tetrahydroindazolone. To address these issues, we aimed to develop a new method to carry out orthogonal regioselective synthesis and facile diversification to obtain complementary regioisomers of N-alkyl-3-substituted tetrahydroindazolone from Boc-protected alkylhydrazines. The key step in this synthesis strategy is the introduction of a protecting group such as Boc at the nitrogen atom of the internal amine in the alkylhydrazine. This causes a difference in the nucleophilicities of the two reactive nitrogens of alkylhydrazines. Consequently, the reaction of the protected alkylhydrazine with 2-acylcyclohexane-1,3-diones and dimedone leads to the regioselective generation of intermediate C and enehydrazine, respectively. We also successfully demonstrated the generality and orthogonality of this synthetic strategy by introducing alkyl or aryl substituents at the C-3 position of 3 and 4; for this purpose, we used various 2-acylcyclohexane-1,3-dione and substituted aldehydes, respectively. This regioselective synthetic method is clearly better than the previously reported methods in terms of robustness and orthogonality

and allows the systematic construction of a small-molecule library that includes privileged tetrahydroindazolone regioisomers obtained in good yields and with excellent regioselectivity.



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장소: 제주ICC

발표코드: ORGN.O-7

발표분야: Oral Presentation for Young Organic Chemists

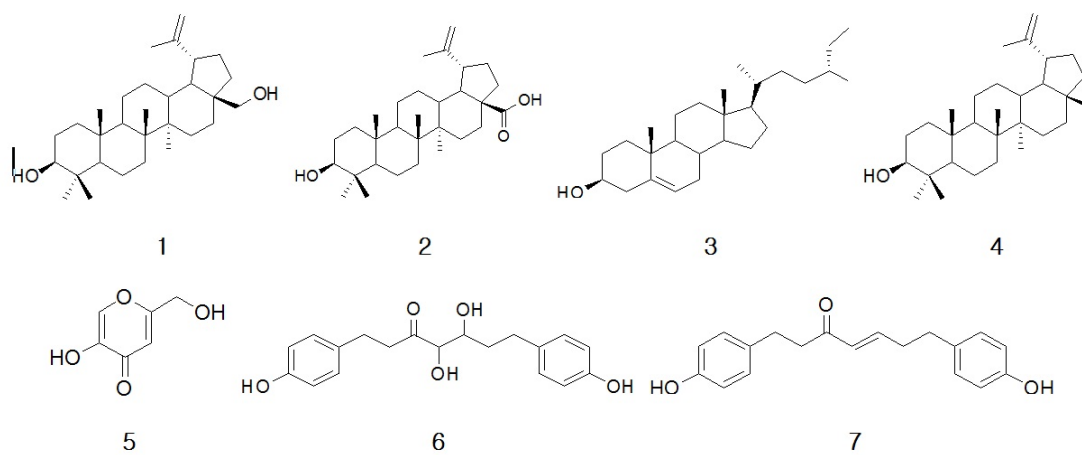
발표종류: 구두발표, 발표일시: 금 10:40, 좌장: 전홍배

Isolation and structure elucidation of bioactive components from *Betula schmidtii*

왕다혜, *정하숙, 고은희

Department of Chemistry, College of Natural Sciences, Duksung Women's University *Department of
Food and Nutrition, College of Natural Sciences, Duksung Women's University

From thousands years ago, wild plants have been used for the treatment of diseases as a folk medicine. As a part of our ongoing study for the identification of biological activity of natural sources, we were investigated the phytochemicals from *Betula schmidtii*. *Betula schmidtii*.(Betulaceae) is commonly used in Korea, Japan and Northern China as a folk medicine. Dried inner bark of *Betula schmidtii* were extracted with 80% ethyl alcohol to give dark yellow extracts. Dried ethanolic extracts were fractionated with *n*-hexane, chloroform, ethyl acetate and *n*-butyl alcohol, respectively to yield solvent-soluble fractions. Seven compounds were isolated from active solvent soluble fractions through silica gel open column and vacuum liquid column chromatographic methods. The chemical structure of compounds were elucidated as betulin (1), betulinic acid (2), β -sitosterol (3), lupeol (4), kojic acid (5), 1,7-bis-(*p*-hydroxyphenyl)-(3,4-dihydroxy)-5-hepanone (6), 1,7-bis(4-hydroxyphenyl)-4-heptene-3-one (7) by spectroscopic study. Compounds 1 and 5, 6 showed neuroprotective and antioxidant activities, respectively.



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장소: 제주ICC

발표코드: **ORGN.O-8**

발표분야: Oral Presentation for Young Organic Chemists

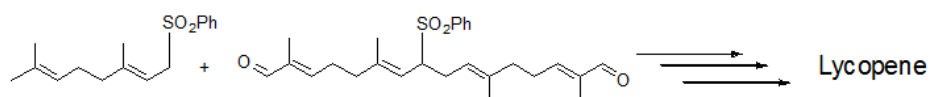
발표종류: 구두발표, 발표일시: 금 10:50, 좌장: 전홍배

A Highly Efficient Synthetic Method of Xanthophyll

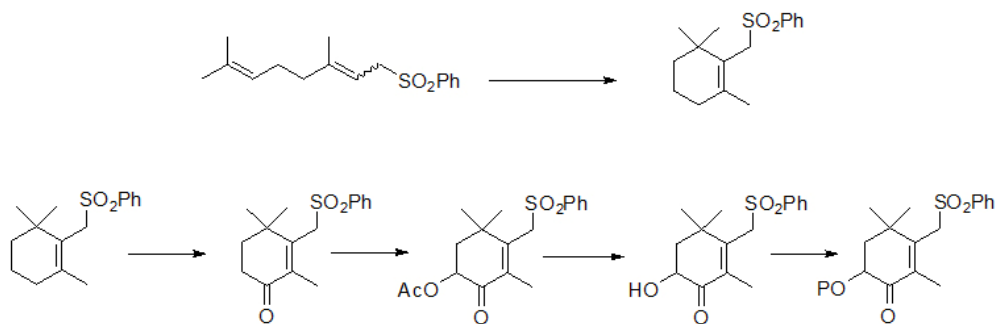
심상은, 구상호

명지대 화학과

Xanthophyll is pigments occurring in the leaves of plants and giving young shoots and late autumn leaves their characteristic color. This color is masked by chlorophyll when the leaf is mature. Xanthophylls are carotenoids, differing from β -carotene in having one or more oxygen-containing groups attached. We have reported a general synthetic method of carotene such as lycopene based on the sulfone coupling and double elimination strategy using C_{20} dialdehyde and Geranylsulfone. So, We applied the above method to prepare astaxanthin. Geranylsulfone is cyclized in $AcOH-H_2SO_4$ to give the cyclic sulfone, which undergoes consecutive oxidation reaction, as shown in the scheme. The resulting hydroxycyclohexenone is used for coupling with the C_{20} dialdehyde. The double elimination method then produced astaxanthin.



Expeditious and Practical Synthesis of Lycopene (Advanced Synthesis & Catalysis 2008, 350, 365-369)



Synthesis of various C10-cyclohexene moiety



일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: **ORGN.O-9**

발표분야: Oral Presentation for Young Organic Chemists

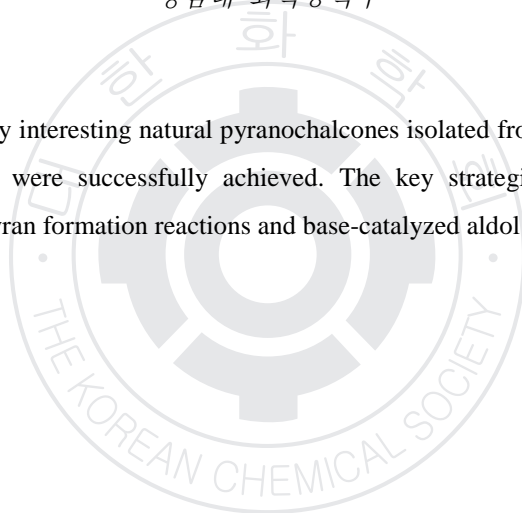
발표종류: 구두발표, 발표일시: 금 11:00, 좌장: 전홍배

Concise Synthesis of Biologically Interesting Pyranochalcones from Mallotus Philippensis and Their Unnatural Derivatives

하렵개, 이용록

영남대 화학공학부

The synthesis of biologically interesting natural pyranochalcones isolated from *Mallotus Philippensis* and their unnatural derivatives were successfully achieved. The key strategies involve ethylenediamine diacetate-catalyzed benzopyran formation reactions and base-catalyzed aldol reactions.



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장소: 제주ICC

발표코드: ORGN.O-10

발표분야: Oral Presentation for Young Organic Chemists

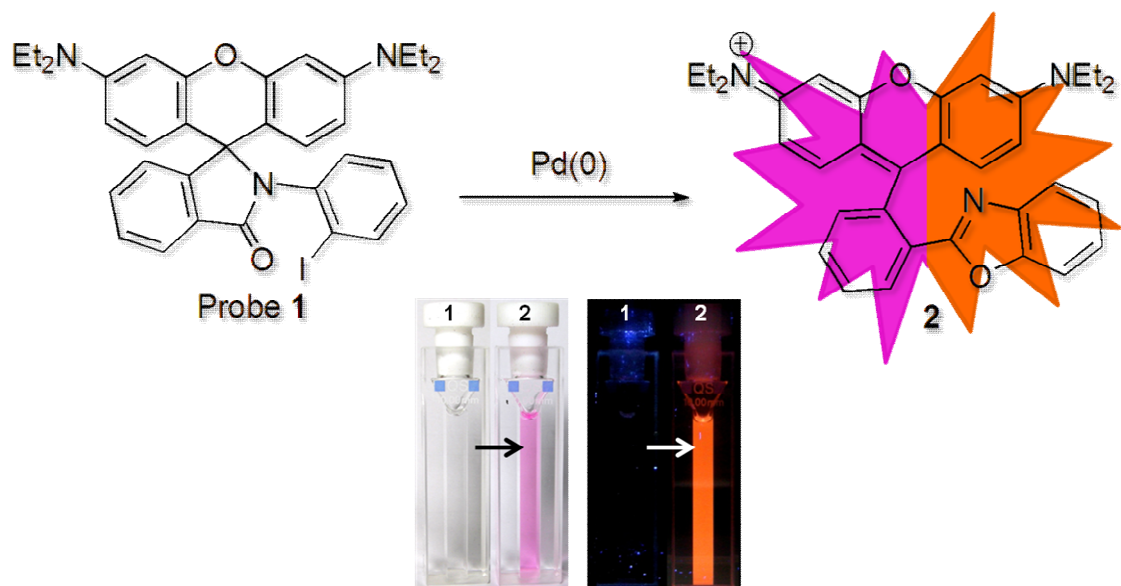
발표종류: 구두발표, 발표일시: 금 11:10, 좌장: 전홍배

A Rhodamine B Derivative for the Reaction-based Fluorogenic and Chromogenic Detection of Pd Species

전미은

포항공과대 화학과

Palladium catalyzed cross-coupling reaction has found an important place in modern synthetic protocols because it can perform to make difficult covalent bond in medicine and materials. However, even after purification, residual palladium is often found in the final product, which may be a health hazard. For that reason, easy detection of palladium species is an important goal.¹ Along with our efforts to develop efficient molecular probes based on organic reactions, we have developed a simple yet efficient detection method for palladium species based on a molecular sensing system that undergoes a palladium catalyzed oxidative addition.² A rhodamine B derivative thus developed undergoes the catalytic process triggered by palladium insertion and gives both turn-on fluorescence and color changes. The catalytic ring-opening process is specific toward palladium species such as PdCl₂ or Pd₂dba₃ in the presence of [(t-Bu)₃PH]BF₄ at 85 °C, among various metal chloride species examined. A usefulness of the sensing system is demonstrated by determining the residual palladium contents in a purified sample prepared through a palladium-catalyzed reaction. This is the first reaction-based sensing system for palladium species that gives both the turn-on fluorescence and color changes. Reference: 1) Song, F.; Garner, A. L.; Koide, K. *J. Am. Chem. Soc.* 2007, 129, 12354. 2) Jun, M. E.; Ahn, K. H. *Org. Lett.* 2010, 12, 2790.



일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: ORGN.O-11

발표분야: Oral Presentation for Young Organic Chemists

발표종류: 구두발표, 발표일시: 금 11:20, 좌장: 전홍배

Energy Transfer Dynamics of [26]/[28]Hexaphyrin-BODIPY hybrids

신지영, *Kil Suk Kim, *Jong Min Lim, **김동호, 김기문

포항공과대 지능초분자연구단, 첨단재료과학부, 화학과 *Department of Chemistry, Yonsei University **연세대 화학과

Multichloromophoric species has been very attractive in their fascinating photochemical and photophysical properties due to their potential for application in the exploration of artificial systems for light harvester and storages. Since the formation of a series of *meso*-aryl substituted expanded porphyrins has been reported in 2001, among the series, hexaphyrins have been most intensively studied due to their high reaction stability. Upon this, a unique system combining hexaphyrin and boron dipyrin (bodipy) was investigated to demonstrate their energy transfer facility for the purpose of energy harvesters. Hexaphyrin exhibits multi-redox behavior with specially two stable oxidation states, [26] and [28]hexaphyrins which are interconversional. While [26]hexaphyrin has distinct aromaticity upon its rigid and planar structure, [28]hexaphyrin exhibits a structurally dynamic mixture of predominant Möbius aromatic structure. We consecutively prepared a novel series to have different center to center distances within the hexaphyrin and the bodipy groups. Energy transfer dynamics within both [26] and [28]hexaphyrin systems showed reliable results, long lived energy transfer excited states increased in accordance with the increase of the center to center distances within the two moieties. Details of the synthesis and characterization will be presented and their photodynamics will be demonstrated in the presentation.

일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: EDEC.O-1

발표분야: Current Trends in Chemical Education: Development of Teachers' PCK (Pedagogical Content knowledge)

발표종류: 구두발표, 발표일시: 금 14:00, 좌장: 장신희

초등 과학영재교육에서 코티칭의 유용성 탐색

강훈식

춘천교육대 과학교육과

이 연구에서는 초등 과학영재교육에서 코티칭의 유용성을 탐색하기 위해, 코티칭 과학영재 수업 과정의 특징을 분석했다. 또한 그 효과를 개념 적용 능력과 수업에 대한 인식 측면에서 조사했다. 초등학교 과학영재학급 5학년 학생 37명을 선정하여 각각 한 명의 교사가 수업을 실시하는 개별 수업 집단과 두 명의 교사가 수업을 실시하는 코티칭 수업 집단으로 배치했다. 두 명의 교사가 코티칭을 활용하여 진행한 12차시의 과학영재수업을 관찰하고, 수업 동영상과 교사들이 작성한 일지 및 교사들과의 심층 면담 전사본 등을 분석했다. 모든 수업이 끝난 후, 두 집단 학생들에게 모두 개념 적용 능력 검사를 실시했고, 코티칭 수업 집단의 모든 학생들에게는 코티칭 과학 수업에 대한 인식 검사를 실시한 후 이에 대한 심층 면담도 실시했다. 연구 결과, 수업 계획 단계에서는 과학영재교육 프로그램의 질 향상과 과학영재교육 프로그램 개발에 대한 심리적 부담감 감소가 코티칭의 특징으로 나타났다. 수업 진행 단계에서 나타난 코티칭의 특징으로는 역할분담을 통한 원활한 수업 진행, 학생들의 탐구 기회 증가, 교사의 미흡한 설명과 간과한 내용의 보완, 교사와 학생 및 학생 간의 상호작용 증가, 실험안전사고의 위험 감소 등이 있었다. 수업 반성 및 평가 단계에서 나타난 코티칭의 특징은 평가 관점의 다양화와 수업 전문성 향상을 위한 배움의 기회 증가로 분류할 수 있었다. 개념 적용 능력 검사 점수에 대한 일원공변량분석 결과, 개별 수업 집단보다 코티칭 수업 집단의 점수가 유의미하게 높았다. 많은 과학영재 학생들이 코티칭 과학영재 수업의 장점에 대해 다양한 측면에서 긍정적으로 인식했으나, 일부 학생들은 몇 가지 단점을 지적하기도 했다. 이에 대한 교육적 함의를 논했다.

일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: EDEC.O-2

발표분야: Current Trends in Chemical Education: Development of Teachers' PCK (Pedagogical Content knowledge)

발표종류: 구두발표, 발표일시: 금 14:30, 좌장: 장신호

용해와 확산에 대한 교과서 서술 분석과 개념 구분

박종윤

이화여대 과학교육과

용해와 확산은 우리 주위에서 쉽게 관찰할 수 있는 현상으로 초등학교에서부터 그 내용이 제시된다. 그러나 선행연구에 의하면 많은 교사와 학생들이 용해와 확산을 서로 구별하지 못한다고 한다. 그러므로 본 연구에서는 용해와 확산을 구별하지 못하는 원인을 알아보고자 교과서의 서술 내용을 분석하였다. 이를 위해 초중고 과학 및 화학 교과서와 대학 일반화학 및 물리화학 교재에서 용해와 확산에 대한 정의를 조사하여 정리하였다. 그 결과 용해는 초등학교와 중학교 교과서에서는 대체로 고르게 섞임 또는 녹아서 고르게 섞임으로 정의하였고, 고등학교 화학 II 교과서에서는 용해의 정의에 대한 서술이 대체로 없었다. 대학교 교재에서는 용액에 대한 정의는 서술되어 있었으나 용해에 대한 정의는 찾아보기 어려웠다. 확산은 중학교, 고등학교 교과서와 대학 일반화학 교재에서 대체로 다른 물질 속으로 스스로 움직여서 퍼져나가는 현상으로 서술하였으며, 농도 차에 의해 이동한다는 설명은 거의 없었다. 반면 대학 물리화학 교재에서는 대부분 농도 차에 의해 입자가 이동한다고 서술하였다. 따라서 초중고 교과서에서 용어에 대한 정확한 정의가 제시되지 않은 것이 두 개념을 분명하게 구별하지 못하는 원인의 하나로 생각되며, 향후 용어의 정의를 명확하게 구분하여 서술하는 것이 필요한 것으로 생각된다.

일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: **EDEC.O-3**

발표분야: Current Trends in Chemical Education: Development of Teachers' PCK (Pedagogical Content knowledge)

발표종류: 구두발표, 발표일시: 금 15:30, 좌장: 장신호

연소에 대한 초등학생의 개념 조사

신애경

제주대 교육대학 초등과학교육전공

연소 개념은 우리나라의 교육과정상 초등학교 6 학년에 처음 다루어지는 내용으로 화학적 변화를 다루기 때문에 학생들이 이해하기 쉽지 않은 개념이다. 따라서 학생들이 연소를 학습한 후 이에 대해 어떻게 이해하고 있는지를 알아보는 것은 새로운 교과서 집필이나 교사용 자료 집필, 또는 교사 연수시 유용한 자료를 제공할 수 있다. 이 연구를 위해 제주도내에 위치한 초등학교 3 개교를 선정하고, 각 학교별로 6 학년 2 개 학급씩 약 150 여명을 연구 대상으로 선정하였다. ‘연소와 소화’라는 단원 학습 직후 연소 개념 검사지를 투입하여, 학생들이 학습 후 연소 개념을 어떻게 형성하고 있는지에 대해 알아보았다. 연소 개념 검사지는 연소의 개념, 집기병으로 덮었을 때 촛불이 꺼지는 이유, 촛불이 꺼질 때 집기병 속의 기체의 종류와 양의 변화, 연소 후 생성물에 대한 문항으로 구성되어 있다.

일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: II-POLY.P-1

발표분야: 고분자화학

발표종류: 포스터, 발표일시: 목 15:00~17:00

Patterning of Various Silicon Structures via Polymer Lithography and Catalytic Chemical Etching

이정필, 최신호, 박수진

울산과학기술대 친환경에너지공학부

Precisely controlled patterns of organics, inorganics, and composites are of great interest in areas of microelectronics and optical devices. We demonstrate a facile fabrication of a rich variety of silicon patterns with different length scales by combining polymer lithography and metal-assisted chemical etching method. Several types of polymer patterns such as concentric circles, squares, and lines were fabricated on silicon substrates by conventional lithography. Moreover, block copolymer self-assembly for surface patterning was introduced to make tens-of-nanometer patterns with higher density, easy process, and low cost. Silver layers were deposited on the patterned silicon surfaces and used to etch the silicon beneath, resulting in generating the corresponding silicon patterns.

일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: II-POLY.P-2

발표분야: 고분자화학

발표종류: 포스터, 발표일시: 목 15:00~17:00

Synthesis of Polymers Including Both Triazole and Tetrazole by Click Reaction

신정아, 임영권

국방과학연구소 4기술연구본부 2부

Triazole and tetrazole compounds have received wide attention by many chemists as energetic materials, pharmaceutical and material sciences. Polymers containing triazole or tetrazole, respectively are well known as energetic materials. While polymers containing triazoles made by click reaction are found easily, polymers containing tetrazole groups such as polyvinyltetrazole are very rare and begin to grab the attention as energetic polymers, recently. Moreover, polymers containing both triazole and tetrazole are not published to date to the best of our knowledge. The non-polymeric compounds containing both triazole and tetrazole are also very rare. We found that polymers containing azido groups converted easily to glycidyl tetrazolyl triazole polymers by the click chemistry. These polymers have good solubility in organic solvents such as CH_2Cl_2 , CHCl_3 and THF. We believe that these polymers are good candidates for high energetic materials.

일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: II-POLY.P-3

발표분야: 고분자화학

발표종류: 포스터, 발표일시: 목 15:00~17:00

Durable polyacrylic adhesives based on their hybrid organic/inorganic nanocomposites with silica

황귀승, 정일두

부산대 고분자공학과

Hybrid organic/inorganic nanocomposites composed of inorganic nanoparticles and polymers are novel and unique class of nanomaterial and can be potentially used in the field of specialty coatings, optics, electronics, and biomaterials. Silica nanoparticles have been used for a variety of applications depending on their size, porosity, and hardness by controlling the interparticle aggregation with the method of chemical modification of the silica surface. In this work, hybrid organic/inorganic nanocomposites were synthesized from well-dispersed spherical silica nanoparticles which were prepared from colloidal silica and methyltrimethoxysilane(MTMS), followed by the incorporation into acryl resin to improve the mechanical properties and durabilities. The size and morphology of the resulting particles were examined by FE-SEM and TEM.

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장소: 제주ICC

발표코드: II-POLY.P-4

발표분야: 고분자화학

발표종류: 포스터, 발표일시: 목 15:00~17:00

Synthesis and characterization of well-defined acrylic 4-arm star polymers

정병진, 정일두

부산대 고분자공학과

Star polymers are a special kind of branched polymers composed of a central core and different numbers of linear chains with the properties of low solution or melt viscosities, because their molecular structures behave similar to a solution of hard sphere and exhibit limited chain entanglements, which is beneficial to polymer processing. The synthesis of 4-arm star polymer had been achieved successfully by atom transfer radical polymerization using n-butyl acrylate(n-BA), methyl methacrylate(MMA), 2-hydroxyethyl methacrylate(HEMA) as acrylic monomers, and pentaerythritol tetrakis(2-bromoisobutyrate) as an initiator. The star polymer was characterized by FT-IR and ¹H NMR spectroscopies and GPC, DSC, respectively.

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장소: 제주ICC

발표코드: II-POLY.P-5

발표분야: 고분자화학

발표종류: 포스터, 발표일시: 목 15:00~17:00

A Simple Route for Fabricating Nanoscale Silicon Hole Structures Using Metal-Assisted Etching.

최신호, *이정필, **박수진

울산국립과학기술대 친환경에너지공학부 *울산과학기술대 친환경에너지공학부 **울산과학기술대 에너지공학부

We have developed a new technique to fabricate a highly ordered silicon hole structure, in which each silicon nanowire is pinned in a hole, by combining polymer sphere arrays induced by Rayleigh instability with chemical etching process. With this process, we were able to create the novel structures that are periodic over very large areas, where the length of silicon nanowires can be varied by tuning the chemical etching time. A silicon hole structure was used as templates for preparing polymer nanotubes. And also these structures exhibited a superior anti-reflection property showing specular reflectance of about 0.1%, nearly three orders of magnitude lower than that of a planar silicon wafer.

일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: II-POLY.P-6

발표분야: 고분자화학

발표종류: 포스터, 발표일시: 목 15:00~17:00

Quasi-solid ion gel membranes for carbon dioxide separation

윤일녕, *박성진, 원종욱

세종대 화학과 *세종대 응용화학과

As global warming has been gradually serious, supported ionic liquid Membrane (SILM) has attracted significant attention, as one of method to separate CO₂. Because of the property of ionic liquid such as high CO₂ solubility and negligible vapor pressure, SILM has been a good candidate as a CO₂ separation membrane. However, in progress of CO₂ separation, since SILM has to be highly pressured, its stability could be ruined by high pressure exceeding capillary force of porous membrane. In order to improve the stability of membrane, tri-block copolymer, poly(styrene-ethylene oxide-b-styrene)(SEOS) was employed, making ion gel. Using three kinds of ionic liquids, [hmim][Tf₂N], [hmim][BF₄], [hmim][PF₆], each ion gel membrane was prepared, and ideal selectivities of them were determined by measuring CO₂ permeance per that of other gases(N₂, CH₄, O₂). To confirm the stability of membrane, we also measured the decay of ideal selectivities of ion gel membranes and SILMs as time flows.

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장소: 제주ICC

발표코드: II-POLY.P-7

발표분야: 고분자화학

발표종류: 포스터, 발표일시: 목 15:00~17:00

Effect of addition of the silicon dioxide nanorod to electrolyte of dye-sensitized solar cell

윤일녕, 송홍규, 원종욱

세종대 화학과

As an alternative of commercial inorganic solar cell, which is too costly, dye-sensitized solar cell (DSSC) has a predominant possibility, due to its economical cost. Because of the high volatility of its liquid state electrolyte which decreases the stability of DSSC, the research into preventing evaporation of electrolyte has been actively proceeded. DSSC using poly(ethylene glycol) dimethyl ether (PEGDME) electrolyte with SiO₂ nanoparticle, performs higher energy conversion efficiency than that without SiO₂ nanoparticle. In this study, we employed SiO₂ nanorod, expecting SiO₂ nano-structure would be a channel of redox couple's movement, under the assumption that, SiO₂ nanorod would help redox couple to diffuse more effectively than SiO₂ nanoparticle. SiO₂ nanorod was prepared by electrospinning method, using tetraethyl orthosilicate and poly vinyl pyrrolidone(PVP). Consequently, DSSC with electrolyte using SiO₂ nanorod was compared with that with electrolyte using SiO₂ nanoparticle.

일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: II-POLY.P-8

발표분야: 고분자화학

발표종류: 포스터, 발표일시: 목 15:00~17:00

Fabrication of Metal Oxide-Assembled Nanoporous Polymer Membranes

정현민, 이지목, *박유주, 현다정, *원종찬, 강준

금오공과대 응용화학과 *한국화학연구원 화학소재단

Nanoporous structures of polymer films, membranes, and composites have received wide attention, due to their usefulness in separation process, separators of energy storage devices, and high surface area catalyst supports. The formations of nanopores through controllable manners in size and connectivity are important criteria for practical uses. In this work, we'll demonstrate the facile approach to form 30 – 200 nm range nanopores with highly inter-connected structures. The method to control pore size, is through 'reversible cross-linking and precipitation', where metal ion induced cross-linking is occurred and swelling polymer-solute matrix is precipitated resulting in porous structures. Also, well developed metal oxides arrays on pore surface from metal ions are obtained, which are observable on TEM images.

일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: II-POLY.P-9

발표분야: 고분자화학

발표종류: 포스터, 발표일시: 목 15:00~17:00

Efficiency Enhancement of Inverted Organic Photovoltaic Cells with High Aspect Ratio ITO Electrode

AN CHENGJIN, *전환진, *최종길, *정희태

KAIST 생명화학공학과 *KAIST 생명화학공학과

We demonstrate inverted organic photovoltaic cells in which nano-patterned ITO electrodes was extended deep within active layer, providing efficient electron transport pathway. The height and diameter of cylinder pattern of ITO electrode fabricated by Second Scattering Lithography(SSL) are 100nm and 400nm respectively. The expected increase of surface area is about 160%. Titanium oxide was uniformly deposited on nano-patterned ITO electrodes by atomic layer deposition(ALD) characterized by excellent conformality on 3-dimensional structure and accurate thickness control with nano-level. Since the conduction band of TiO₂ is similar to that of PCBM, electrons can transport to ITO electrode with ease. Moreover, the valence band of TiO₂ is efficient to inhibit back electron or hole transfer with its high-energy barrier. Therefore, the performance of inverted organic photovoltaic cells ,which are based on the regioregular poly(3-hexyothiophene) and C61 butyric acid methyl ester bulk heterojunction, can be dramatically improved by both shorter traveling distance for electron and the special functional layer of TiO₂, as well as current density.

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장소: 제주ICC

발표코드: II-POLY.P-10

발표분야: 고분자화학

발표종류: 포스터, 발표일시: 목 15:00~17:00

Synthesis of Polymer Nanocage Structure via ATRP and “Click” chemistry

이루다, 백현종

부산대 고분자공학과

Diverse polymer architectures have been attracting attention over the last few decades, because properties of polymer are related to their molecular structure. Recently, synthetic routes for the macrocyclic polymers have been explored via “Click” cyclization of α,ω -difunctional linear precursors. However, there has been no report on polymer nanocage structures using three-arm star polymer. In this study, we synthesized novel structure “Polymer nanocage” using atom transfer radical polymerization (ATRP) and “Click” coupling chemistry. Three-arm star polystyrene polymer ((PS-Br)₃) were prepared by ATRP using tri-functional initiator 1,1,1-Tris(2-bromoisobutyryloxymethyl)ethane and azidation of end group was carried out ((PS-N₃)₃). Trialkyne coupling agent 1,1,1-Tris(ethynylloxymethyl)ethane was synthesized. To synthesize polymer nanocage structures, we used the “Click” reaction between an azido-terminated PS ((PS-N₃)₃) and alkyne-containing trifunctional coupling agent. Molecular weight (MW), molecular weight distribution (PDI), and the degree of polymerization (DP_n) of polymer were determined by gel chromatography (GPC), gas chromatography (GC) and ¹H NMR spectroscopy. The synthesized polymer nanocage structures were characterized by GPC and matrix-assisted laser desorption/ionization-time of flight mass spectroscopy (MALDI-TOF).

일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: II-POLY.P-11

발표분야: 고분자화학

발표종류: 포스터, 발표일시: 목 15:00~17:00

Dispersion of the Single-Walled Carbon Nanotubes Using Poly[2-(Dimethylamino)Ethyl Methacrylate]-*co*-Polystyrene

김동현, 백현종

부산대 고분자공학과

The single-walled carbon nanotubes (SWNTs) coatings on plastic film have been investigated as transparent conductive film (TCF) to alternate indium tin oxide (ITO) electrode. One of important factor that makes TCF more conductive is the dispersion of SWNTs. However, SWNTs exist as a bundle due to a strong intertube van der Waals attraction. In order to obtain well dispersed SWNTs, efficient dispersants are firstly required. In this study, poly[2-(dimethylamino)ethyl methacrylate]-*co*-polystyrene (PDMAEMA-*co*-PS) was synthesized and used as polymeric dispersants for SWNTs in organic solvent. PDMAEMA-*co*-PS with different copolymer composition were prepared by atom transfer radical polymerization (ATRP) and characterized by gel permeation chromatography (GPC) and ¹H NMR. With PDMAEMA-*co*-PS, SWNTs were effectively dispersed through non-covalent functionalization by ultrasonication in tetrahydrofuran (THF). Unbundled structures of SWNTs were observed by transmission electron microscopy (TEM). Using the turbiscan optical analyzer, dispersion stabilities of SWNTs were compared in THF with PDMAEMA-*co*-PS in different copolymer composition. SWNTs coatings on polyethylene terephthalate (PET) film were prepared via spin coating of SWNTs dispersion solution and networks of SWNTs were observed by field emission scanning electron microscope (FE-SEM). Transmittance and sheet resistance of SWNTs coatings were obtained by UV-vis spectroscopy and four point probe measurement, respectively

일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: II-POLY.P-12

발표분야: 고분자화학

발표종류: 포스터, 발표일시: 목 15:00~17:00

Synthesis and Characterization of Comb-Coil Type Block Copolymers via an "Graft-Through" Approach

허재원, 김상율

KAIST 화학과

Comb-coil type block copolymers were synthesized by sequential reversible addition-fragmentation chain transfer polymerizations of methyl methacrylate and macromonomers containing photoresponsive azobenzene units in the side chains. The designed macromonomer was obtained after proper end group modification from PAEAz synthesized through chain-growth condensation polymerization (CGCP). Details on synthetic methods and characterization of the block copolymers will be presented.

일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: II-POLY.P-13

발표분야: 고분자화학

발표종류: 포스터, 발표일시: 목 15:00~17:00

Self-assembly of benzamide containing photo-responsive molecules

김지성, 서명은, 김상율

KAIST 화학과

Benzamide is one of supramolecular synthons which provide two-dimensional hydrogen bonding networks by self-complementary hydrogen bonding. Here we report self-assembly of the benzamide compounds containing a diacetylene group that polymerize under UV radiation. A series of benzamide containing photo-responsive molecules were synthesized and characterized. Self-assembly of the synthesized compounds, especially gelation, in various organic solvents will be discussed.

일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: II-POLY.P-14

발표분야: 고분자화학

발표종류: 포스터, 발표일시: 목 15:00~17:00

Multicolor Emission of Triphenylamine-Based Condensation Polymer

이진희, 허재원, 김상율

KAIST 화학과

Many triphenylamine derivatives have been widely investigated and applied in various electro-optical materials. We synthesized AB type triphenylamine monomer for polymerization via nucleophilic aromatic substitution (SNAr) reaction. Moreover, by introducing the electro withdrawing groups (EWGs) into the triphenylamine, the photo luminescence (PL) was efficiently tuned by the strength of intramolecular charge transfer (ICT). Detailed synthesis and properties of the polymer will be present.

일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: II-POLY.P-15

발표분야: 고분자화학

발표종류: 포스터, 발표일시: 목 15:00~17:00

Slide coating을 이용한 3차원 광결정 구조의 빠른 제작 방법

김슬기, 한성구, 이원목

세종대 화학과

현재 잘 쌓인 colloidal crystal 의 3 차원적인 구조는 다양한 광결정 소자 분야에서의 응용가능성 때문에 그 연구가 활발하다. 최근에 우리는 submicron 크기의 200~300nm PS particles 를 이용하여 빠르고 대면적으로 colloidal crystal film 을 제작할 수 있는 slide coating 방법에 대해 보고하였다. 이번 연구에서는 colloidal crystal film 의 좀더 실용적인 응용을 향한 slide coating 기술 확장을 위해 기존의 coating 방법을 변형시켰다. 새로운 slide coating 방법을 통해서 알코올에 분산된 고분자 입자를 다양한 기판 위에 코팅하였고, Colloidal crystal films 의 잘 쌓인 구조는 SEM 과 reflectance spectra 를 통해서 확인하였다.

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장소: 제주ICC

발표코드: II-POLY.P-16

발표분야: 고분자화학

발표종류: 포스터, 발표일시: 목 15:00~17:00

Various Photonic Crystal pH Sensors Based on Templated Photo-Polymerization of Hydrogel Inverse opal

한성구, 이원목

세종대 화학과

최근 광결정을 응용한 발광소자, 에너지 변환장치 등이 보고되고 있는 가운데, 광결정을 기반으로 한 자극-반응형 하이드로젤 센서도 많은 관심을 끌고 있다. 하이드로젤 센서는 복잡하고 정밀한 전기 화학적 검출법에 비해 자연광의 회절현상을 이용하여 쉽게 육안으로 검출 물질을 sensing 할 수 있다. 그 원리는 pH, 온도, 그리고 chemical molecules 등의 외부 자극에 의해 따른 체적이 변하게 되어 Bragg's law 의 원리에 의해 바뀌는 회절광에 의한 색의 변화로 센서로서 작용하게 된다. 중합 가능한 vinyl 기가 있는 building block 과 가역적으로 binding 할 수 있는 sensing moiety 만 있으면 원하는 검출 물질을 쉽게 sensing 할 수 있는 하이드로젤 센서를 제작 할 수 있다. 따라서 적합한 조합만 찾아 낸다면 원하는 센서를 어렵지 않게 제작할 수 있으며 색의 변화를 관찰 하므로써 쉽게 sensing 할 수 있다. 본 연구에서는 다양한 protic vinyl monomer 들을 가지고 pH 센서를 제작하여 넓은 pH 변화에 대해 다양한 구조색의 변화를 나타내는 pH 센서를 탐구하였다.

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장소: 제주ICC

발표코드: II-POLY.P-17

발표분야: 고분자화학

발표종류: 포스터, 발표일시: 목 15:00~17:00

Synthesis of Graphene Nanocomposites Armed with Nanoneedles; Towards a Poison-Transformer Nanocatalyst

남보라, 고희아, *이하진, *최원산

충남대 분석과학기술대학원 *한국기초과학지원연구원 전주센터

Recently, iron oxide nanoparticles have been extensively studied as drug carriers, contrast agents, heating mediators, and catalysts in many industrial processes. The particle size of iron oxide is a critical factor for almost all of the aforementioned applications. By such reasons, controlled growth of iron oxide NPs is a priority for advanced applications. Au NPs were homogeneously synthesized on graphene via adsorption and reduction of corresponding precursors, and used as catalytic template for growth of iron oxide. We found that iron oxide NPs remarkably grow into needlelike structures on Au NP-coated graphene due to catalytic synergy effect of Au NPs and functionalized carbons, compared to graphene. Growth of iron oxide NPs on templates could be easily tuned by controlling the size and quantity of Au NPs on graphene. Such graphene-derivatives showed excellent performance for chemo-selective reduction of nitrobenzenes to their respective anilines under room temperature.

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장소: 제주ICC

발표코드: II-POLY.P-18

발표분야: 고분자화학

발표종류: 포스터, 발표일시: 목 15:00~17:00

Polyelectrolyte Multilayer-Mediated Chemical Reactor for Hierarchical Nanomaterials with Controllable Properties

고혜아, 남보라, *이하진, *최원산

충남대 분석과학기술대학원 *한국기초과학지원연구원 전주센터

Specially designed structures as chemical microreactors were prepared for synthesizing nanomaterials with tunable properties. Overall structures were microcapsules containing a movable polymer core, referred to as a core-in-shell particle. The Au NP-embedded polymer core-in-SiO₂ shell structures were formed by controlled heat treatment of PEMPR-Au/SiO₂. (PEMPR; polyelectrolyte-coated melamine-formaldehyde particles). After calcination of PEMPR-Au/SiO₂, gold nanoparticles (NPs) with high mobility under such conditions were homogeneously distributed on certain region of polymer particles and it led to the transformation of polymer particles. Selective dissolution of shell materials was able to collect the desired products such as polymer cores. The structures and properties of the metal NP-embedded polymer cores could be also tuned by varying the metal NPs which possess different thermal properties. Among the product materials, Au NP-embedded polymer cores were effectively utilized as nanocatalysts for transformation of 4-nitrophenol to 4-aminophenol. Our approach might be further used for tuning the structures and properties of all kinds of polymer matrices.

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장소: 제주ICC

발표코드: II-POLY.P-19

발표분야: 고분자화학

발표종류: 포스터, 발표일시: 목 15:00~17:00

Synthetic Sugar-based Polyamides for Biomedical Applications

정근수, *김세훈, **박종래

서울대 재료공학부, KIST 의과학센터 *KIST 의과학센터 **서울대 재료공학부

The advent of new polymeric materials has been demanded over the past decade to overcome the instability of therapeutic agents in physiological condition. Polyethylene glycol (PEG) has been recognized as a promising material to improve the bioavailability of drugs by acceptable biocompatibility, less toxicity, and characteristic anti-fouling effect. However the utility of PEG for widening the application areas has been limited, since it does not have reactive functional groups on its main chain, thus the chemical modification is allowed only at the chain ends.. Here we report novel synthetic sugar-based polyamides (SPA) as an alternative to PEG. Galactaric acid (GA), a natural monosaccharide diacid containing four hydroxyl groups, was polymerized with oligo-ethylene oxide (EG) diamines, to produce hydroxyl-rich polyamides with combined functionalities (additional backbone modification at GA units and an anti-fouling effect induced by oligo-EG units). The anti-fouling effect was confirmed by examining the cell attachment behavior to the plate surface treated with SPA and the biodistribution after intravenous injection of SPA solution to the mouse model. Further, the cell-SPA interaction could be controlled by direct conjugation of folic acid (a targeting moiety) to GA units in the backbone, suggesting potential uses of pendant hydroxyl groups as a chemical attaching point.

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장소: 제주ICC

발표코드: II-POLY.P-20

발표분야: 고분자화학

발표종류: 포스터, 발표일시: 목 15:00~17:00

H-bond assisted ROMP from the secondary amide of 1-substituted cyclobutene

이길선, 최태림

서울대 화학부

The ROMP of the secondary amides of 1-substituted cyclobutene exhibits the optimal level of reactivity by polymerization using Grubbs 3rd generation catalyst $[\text{RuCl}_2(\text{IMesH}_2)(3\text{-ClPy})_2(=\text{CHC}_5\text{H}_5)]$. The secondary amides provide regioregular polymers with E-olefin geometry. Here, we propose that the hydrogen of the secondary amides may interact with the carbonyl oxygen of an incoming monomer through H-bonding, which directs a monomer efficiently to the ruthenium carbene center. To prove involvement of H-bonding to initiation rate, NMR tube kinetic experiments were conducted using various solvents (DCM, THF, and toluene) and benzoic acid as an additive. Polymerization in toluene, an optimal solvent, was approximately 2 times faster than those in other solvents within less than 1h to reach 100% conversion.

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장소: 제주ICC

발표코드: II-POLY.P-21

발표분야: 고분자화학

발표종류: 포스터, 발표일시: 목 15:00~17:00

Synthesis of rod-like polymer via ROMP

김경오, 최태림

서울대 화학부

Entangled structure is intrinsic property in most polymers. For the broader application on material science, this structural limitation should be overcome. In this study, dendron was introduced as a solution because it has bulky structure which is possible to control the linearity of polymer chain. Dendronized polymers based on norbornene were synthesized via ring opening metathesis polymerization using ruthenium catalysts. The molecular weight and PDI were determined by GPC, and the structural characterizations were conducted by NMR and AFM imaging. The polymers derived from the monomer which is containing high generation of dendrons (G4 and G5) show good linearity and $M_n=110\text{kDa}$, $\text{PDI}=1.08$. It is expected to be applied on material science, especially in electronics.

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장소: 제주ICC

발표코드: II-POLY.P-22

발표분야: 고분자화학

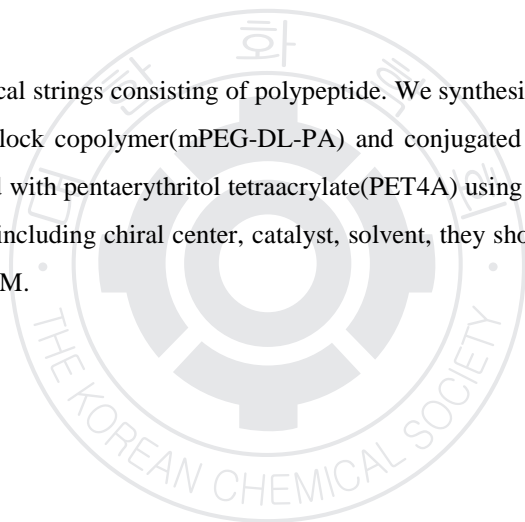
발표종류: 포스터, 발표일시: 목 15:00~17:00

Helical strings consisting of polypeptide in nonchiral environment

박수현, *최보규, *주민경, **박민희, *문효정, *정병문

이화여대 바이오융합과학과 *이화여대 화학나노과학과 **이화여대 나노과학부

We are reporting about helical strings consisting of polypeptide. We synthesized a methoxy poly(ethylene glycol)-DL-polyalanine diblock copolymer(mPEG-DL-PA) and conjugated with methacryloyl chloride. Then, they were crosslinked with pentaerythritol tetraacrylate(PET4A) using APS/TEMED. Though there was no chiral environment including chiral center, catalyst, solvent, they showed helical structures. They were investigated by FE-SEM.



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발표분야: 고분자화학

발표종류: 포스터, 발표일시: 목 15:00~17:00

Thermal gel of chitosan-g-(PA-PEG) aqueous solution and its biodegradation and histocompatibility study

강은영, 윤은정, 연보라, 정소영, *정유경, *정병문

이화여대 바이오융합과학과 *이화여대 화학나노과학과

We are reporting a PEG-PA grafted chitosan(CS-g-(PA-PEG)) as a new temperature sensitive reverse thermal gelling polymer system. With the introduction of PA with α -helical structures between chitosan and PEG, the gel modulus is expected to be increased, compared with previous chitosan-based thermal gel. The CS-g-(PA-PEG) was characterized using NMR, FTIR, SEM, and CD. Thermal properties were investigated by test tube inverting method and Rheometer. In addition, the biodegradability and histology were also studied to confirm the potential of CS-g-(PA-PEG) as a promising biomaterial for use in DDS.

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장소: 제주ICC

발표코드: II-POLY.P-24

발표분야: 고분자화학

발표종류: 포스터, 발표일시: 목 15:00~17:00

Preparation of a flexible and ductile Poly(lactic acid)

배재연, 김미란, *박병식, 윤근병

경북대 고분자공학과 *한국국제대 제약공학과

Melt blending of polylactic acid (PLA) and a chain-extended polyethylene glycol (CE-PEG) have been performed in an effort to toughen the PLA without significant loss of modulus and ultimate tensile strength. The chain-extended PEG was prepared with melt condensation of a low molecular weight PEG and 4,4'-methylenebis-(phenylisocyanate) (MDI) for enhancement of the molecular weight of PEG. Melt blending of PLA and thermoplastic polyester elastomer (TPEE) has been performed in an effort to toughen the PLA. In order to enhance the compatibility of PLA and TPEE, a diisocyanate compound was used as a reactive modifier. The thermal and mechanical properties, miscibility and phase morphologies of the blends were investigated.

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장소: 제주ICC

발표코드: II-POLY.P-25

발표분야: 고분자화학

발표종류: 포스터, 발표일시: 목 15:00~17:00

염료감응 태양전지 전해질 내의 polyrotaxane 이온 채널 도입의 효과

송홍규, 원종욱

세종대 화학과

염료감응 태양전지의 안정성 및 내구성 향상을 위해 고체상 및 준고체상 전해질을 이용하였다. 이에 따른 고체상 전해질 염료감응 태양전지의 에너지 변환효율 향상을 위해 α -cyclodextrin 을 이용하여 polyrotaxane 을 합성하고 이를 이용한 이온채널을 만들어 고체상 전해질에 적용하였다. 고체상 전해질의 낮은 이온 전도도를 높이기 위해서는 채널간 연결성이 좋아야 하기 때문에 α -cyclodextrin 의 특성을 이용하였다. Polyoxyethylene bis(amine)과 α -cyclodextrin 포화 용액을 사용하여 pseudopolyrotaxane 을 합성하고, 이와 dinitrofluoro benzene 을 혼합하여 polyrotaxane 을 제조한 후, polyrotaxane 과 epichlorohydrin 을 반응시켜 이온채널을 생성하였다. 이를 고체상 전해질에 도입하여 염료감응 태양전지를 제작하였다. 이에 따른 결과를 확인하기 위해 photovoltaic performance 의 측정을 통해 향상된 에너지 변환효율을 확인할 수 있었고, EIS 와 IMVS, 그리고 IPCE 를 이용하여 에너지변환 효율에 미치는 영향을 연구하였다.

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장소: 제주ICC

발표코드: II-POLY.P-26

발표분야: 고분자화학

발표종류: 포스터, 발표일시: 목 15:00~17:00

알콕시실란계 석재 강화제의 반응속도에 따른 함침성 및 특성 변화 연구

박성진, *원종욱

세종대 응용화학과 *세종대 화학과

풍화된 석재 조직의 응집력을 주어 강화시키는 것뿐만 아니라, 물의 침투로 인하여 발생될 수 있는 석재의 손상을 막기 위하여 개발된 1:1 몰 비의 tetraethoxysilane 및 3-glycidoxypentyl-trimethoxysilane 혼합물로 이루어진 기능성 강화제의 발수성과 침투성을 향상시키기 위한 연구를 진행하였다. 수분은 석재의 기공에 침투하여 손상시키기 때문에 석조문화재의 주요 박리 및 박락의 원인이 된다. 본 연구에서는 소수성 치환기를 가지는 methyltriethoxysilane 와 ethyltriethoxysilane 을 강화제에 첨가하여 발수특성이 강화되도록 하였다. 또한, 강화제의 경화 반응시간을 늦추어 동일 경화시간 내에 석재 표면으로의 함침량을 증대시키기 위해 경화반응의 촉매인 염산과 dibutyltin diacetate 를 다양한 농도로 변화시켜 제작하고, 대표적인 문화재용 석재인 화강암 시편에 개발한 강화제들을 직접 도입하였다. 처리된 시편을 물에 장시간 담가 무게 변화량과 표면에서 물의 접촉각을 측정하여 강화제의 함침성증가 및 발수성증가를 확인하였으며, 시편의 압축강도를 초음파 탐상장비를 이용, 측정하였다. 각 시료를 표준상태에서 경화시키고 무게감소측정과 FT-IR spectrum 을 이용하여 경화 시간을 정하였으며, 형성된 젤의 물리적 특성을 관찰하였다.

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장소: 제주ICC

발표코드: II-POLY.P-27

발표분야: 고분자화학

발표종류: 포스터, 발표일시: 목 15:00~17:00

Ion Gel Electrolyte와 Dendron을 이용한 염료감응 태양전지의 연구

윤진선, 원종욱

세종대 화학과

Dye-sensitized Solar Cell (DSSC)의 전해질 성능 연구에서 ion gel electrolyte (IGE)는 낮은 광전환효율의 구현에도 불구하고 낮은 휘발성과 누액현상을 막을 수 있다는 장점을 가지고 있다. 따라서 ABA 형태의 triblock copolymer 인 poly(styrene-b-ethylene oxide-b-styrene)를 첨가하여 IGE 를 제작한 후 이를 DSSC 에 적용하였다. 또한 TiO_2 표면에 염료가 흡착되어 있지 않은 공극에 공흡착제를 흡착시켜 효율 저하의 주요원인인 recombination 을 제어해 보는 연구를 진행하였다. 흡착제로는 TiO_2 표면에 흡착하기 위한 표면기능기를 가진 가지구조의 Dendron 을 사용하였다. IGE 의 효과와 공흡착제의 처리 전후의 J_{sc} 및 광전환효율의 변화를 확인하기 위하여 J-V characteristics 를 측정하였으며 EIS, IPCE, IMVS 를 통해 전기화학적 분석을 하였다.

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장소: 제주ICC

발표코드: II-POLY.P-28

발표분야: 고분자화학

발표종류: 포스터, 발표일시: 목 15:00~17:00

UV에 의해 광중합되는 전해질을 이용한 염료감응형 태양전지의

특성 연구

박성진, 원종욱

세종대 화학과

염료감응형 태양전지에서 액체상 전해질의 높은 휘발성과 누액현상을 보안하기 위하여 개발된 polymer gel electrolyte (PGE)는 높은 열적, 물리적 안정성을 갖지만 학계에 알려진 약 11%의 광전환효율을 달성하지는 못한다. 이는 PGE 가 갖는 고체상 특유의 낮은 전자이동도와 dye 표면에서 접촉면적의 감소가 일어나 광전환효율이 감소한 것으로 예상된다. 이러한 접촉면적의 감소는 액체상 전해질을 dye layer 에서 직접 gelation 하는 것으로 극복할 수 있을 것이다. 본 연구에서는 이러한 액체전해질과 PGE 의 단점을 모두 극복하기 위해 UV 광에 의해 젤화되는 poly(ethylene glycol) diacrylate 를 각기 다른 분자량($M_n=258, 575$)으로 이용하여 electrolyte 를 제작하고, 이를 염료감응형 태양전지에 응용하여 광전환효율 및 다양한 열적, 물리적, 전기화학적 특성을 비교 연구하였다.

일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: II-POLY.P-29

발표분야: 고분자화학

발표종류: 포스터, 발표일시: 목 15:00~17:00

Development of various PS-b-P4VP micellar morphologies: Fabrication of inorganic nanostructures from micellar templates

조희숙, *박수진

울산과학기술대 친환경에너지공학부 *울산과학기술대 에너지공학부

We demonstrate a simple route for preparing various micellar nanostructures, like spheres, cylinders, and vesicles, by spin-coating or drop-casting process of polystyrene-block-poly(4-vinylpyridine) (PS-b-P4VP) copolymer solutions in pure tetrahydrofuran (THF), THF/water, and THF/ethanol mixture. Upon drying, solvent selectivity plays an important role in determining micellar nanostructures in thin films. In solution, micellar sizes and shapes of these PS-b-P4VP copolymers were investigated by dynamic and static light scattering. Immediately after spin-coating the polymer solutions, surface and internal morphologies of the films were observed by atomic force microscopy and transmission electron microscopy. As the polymer concentration in THF or the amounts of water or ethanol added in THF solutions was varied, a remarkable difference in the PS-b-P4VP micellar morphologies was observed, from which spherical or cylindrical or vesicular micelles were developed. These micellar films were used as scaffolds or templates for fabricating metal nanodots or nanowires arrays.

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장소: 제주ICC

발표코드: II-POLY.P-30

발표분야: 고분자화학

발표종류: 포스터, 발표일시: 목 15:00~17:00

Enhancement of Physical Properties of Thermoplastic Polyether-ester Elastomer (TPEE) by Reactive Extrusion with Chain Extender

채성민, *조은혜, *윤근병

경북대 대학원/고분자공학과 *경북대 고분자공학과

The branched thermoplastic polyether-ester elastomer (TPEE) and diisocyanate compound was melt extruded in an effort to enhance melt viscosity for the blow molding process. The chain-extended TPEE was prepared with melt condensation of a branched TPEE and 4,4'-diphenylmethane diisocyanate (MDI) for enhancement of the molecular weight of TPEE. The effects of MDI contents as a chain extender on melt, thermal, mechanical and rheological properties of the chain-extended TPEE were investigated. By using a solution and melt viscosity analysis, the chain-extended TPEE was found to be an enhancement of molecular weight and a lightly cross-linked structure. And it has more suitable melt and rheological properties for the blow molding processes

일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: II-POLY.P-31

발표분야: 고분자화학

발표종류: 포스터, 발표일시: 목 15:00~17:00

Reduced Ionic Channel Size of sPES Block Copolymers by Terminal Crosslinking and Its Effect on Proton Conductivity

roshni, 김태현

인천대 화학과

Thermally crosslinkable block copolymers containing sulfonated fluorenyl group with a block lengths of 15.0 Kg/mol (SBCP-1) and 2.0 Kg/mol (SBCP-2) have been successfully prepared and were crosslinked in the presence of bis(aryl azide) as a crosslinker. The AFM showed a microphase separated morphology for the resultant polymers, and a slight reduction in ionic channel size for the crosslinked membranes compared to the non crosslinked counterparts. At 100% R.H., the crosslinked block copolymer having a larger ionic channel size (~ 6.29 nm) showed a higher proton conductivity than the one with smaller channel (0.093 S/cm for SBCP-1 and 0.05 for SBCP-2 at rt), whereas the inversed result was observed at 95% R.H. The higher conductivity for the crosslinked membrane at low R.H. is ascribed to the capillary condensation of water in the ionic channel, which is narrower for the crosslinked membrane than its non-crosslinked counterpart. The experimental details will be presented.

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장소: 제주ICC

발표코드: II-POLY.P-32

발표분야: 고분자화학

발표종류: 포스터, 발표일시: 목 15:00~17:00

Novel Soluble Donor-Acceptor type Conjugated Polymers: synthesis and properties

Mithrabinda, 김태현

인천대 화학과

Donor-acceptor type conjugated polymers have gained much attention in organic electronics due to their unique intramolecular charge transfer and hence narrow band gap. We report herein the synthesis and characterization of new donor-acceptor type semiconducting polymers with a e-rich thiophene and e-poor cyclic ester units. The prepared polymers were readily soluble in most organic solvents and were fully characterized by various spectroscopic methods. The electronic and optical properties of these polymers are currently under investigation. The detailed experiments and properties will be presented.

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장소: 제주ICC

발표코드: II-POLY.P-33

발표분야: 고분자화학

발표종류: 포스터, 발표일시: 목 15:00~17:00

Synthesis, characterization and photovoltaic properties of a low band gap polymer based on Phenothiazine units and cyclopenta[2,1-b:3,4'b']dithiophene

조은혜, 윤근병

경북대 고분자공학과

Conjugated polymeric semiconductors possessing delocalized p-electron systems have potential applications such organic optoelectronic devices as light-emitting diodes (LEDs), organic field effect transistors (OFETs), and photovoltaic cells (PVCs). Many studies of polymer PVCs have focused on optimizing the configuration of the bulk heterojunctions. We report here the Bulk heterojunction solar cells based on blends of photoactive layers of Phenothiazine units and Thiophene derivatives, Poly{3,7-(10-hexyl-10H-phenothiazine)-alt-4,7-(benzo[c][1,2,5]thiadiazole)-2,6(4,4-bis(2-ethylhexyl)-4H-cyclopenta[2,1-b:3,4-b']dithiophene} (P1H) and Poly{1,5-(4,8-dioctoxybenzo[1,2-b:4,5-b']dithiophene-alt-4,7-(benzo[c][1,2,5]thiadiazole)-2,6(4,4-bis(2-ethylhexyl)-4H-cyclopenta[2,1-b:3,4-b']dithiophene} (P3H), acting as electron donor, and [6,6]-phenyl-C71-butyric acid methylester (PCBM), acting as electron acceptor, were constructed and studied. P1H and P3H were synthesized by Suzuki coupling reaction, and characterized UV vis, and photoluminescence spectroscopy.

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장소: 제주ICC

발표코드: II-POLY.P-34

발표분야: 고분자화학

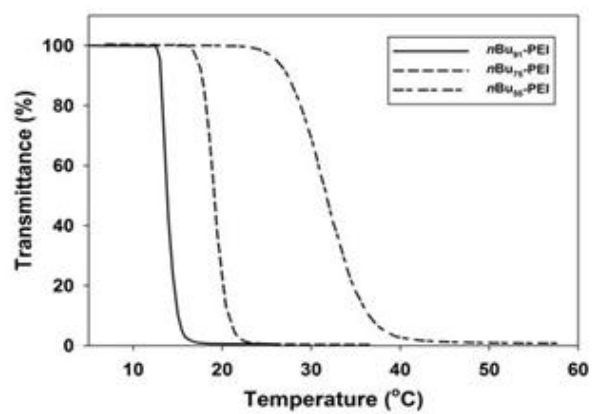
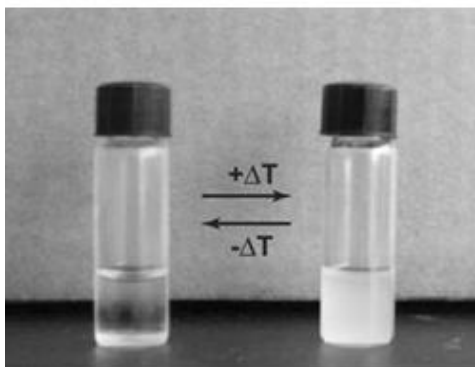
발표종류: 포스터, 발표일시: 목 15:00~17:00

Thermosensitivity control of N-acylated polyethylenimine derivatives

김희진, 이선주, 노민우, 목영봉, 이연

서울대 화학부

Thermosensitive polymers show a hydrophilic to hydrophobic phase transition above a certain temperature, lower critical solution temperature (LCST). Many thermosensitive polymers, such as poly(N-isopropylacrylamide) (PNIPAAm), poly(N-substituted acrylamide)s, poly(N-alkyloxazoline)s, amphiphilic block copolymer, etc. have been intensively investigated for various applications. However, synthetic procedure of existing thermosensitive polymers is usually complicated, so that simpler and easier method to obtain thermosensitivity is required. Because the thermoresponsivity is developed by delicate balance between the hydrophilicity of polar moiety and the hydrophobicity of nonpolar moiety, we expected that a thermosensitive polymer can be synthesized by an introduction of hydrophobic amide groups into a hydrophilic polymer. We obtained thermosensitive polymers by introducing a variety of hydrophobic amide groups into an amine-rich hydrophilic polymer, branched polyethylenimine (b-PEI). The thermosensitivity can be controlled by the hydrophobicity of the acyl groups and the degree of acylation and dependence of the thermosensitivity on pH and ionic concentration. The LCST of N-acyl b-PEI derivatives decreased as the acylation degree increased. Also, lower LCST was shown as the hydrophobicity of the acyl groups increased. Moreover, N-acyl b-PEI contains tertiary amines that can be protonated at acidic pH, so that the LCST transition was observed at elevated temperatures due to the increase of hydrophilicity by the protonation in the acidic environment. General decrease of the LCST was observed as the ionic strength of the solution increased, probably due to the dominance of salting-out effect. In this way, we can successfully obtain N-acyl b-PEI derivatives with temperature- and pH-sensitivity. The N-acyl b-PEI is expected to be useful for biomedical applications requiring more complex signal responsiveness. The very simple introduction of thermosensitivity into a pre-existing polymer can be applied easily into the development of other polymer system with different multiple signal-sensitivities.



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발표코드: II-POLY.P-35

발표분야: 고분자화학

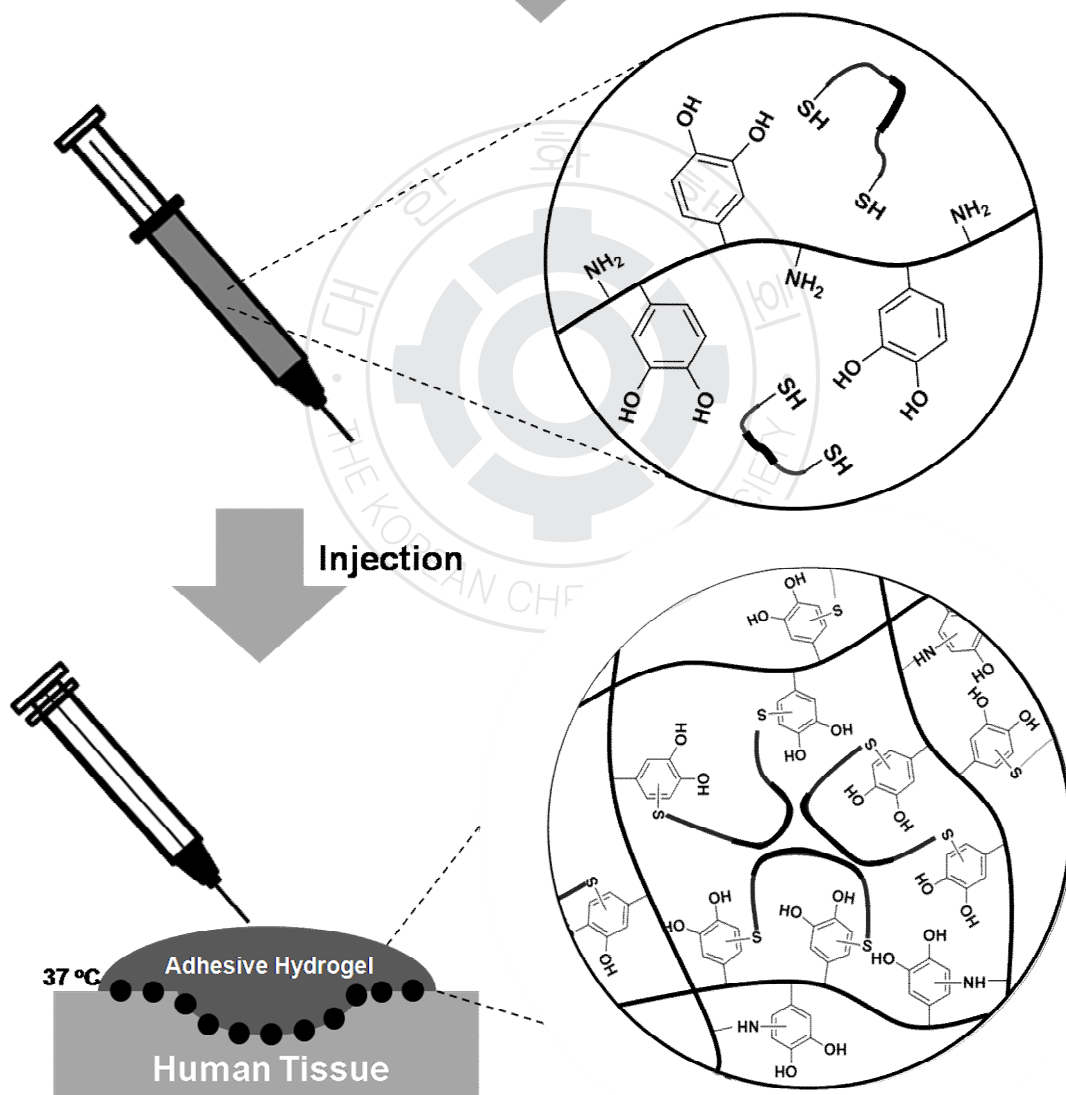
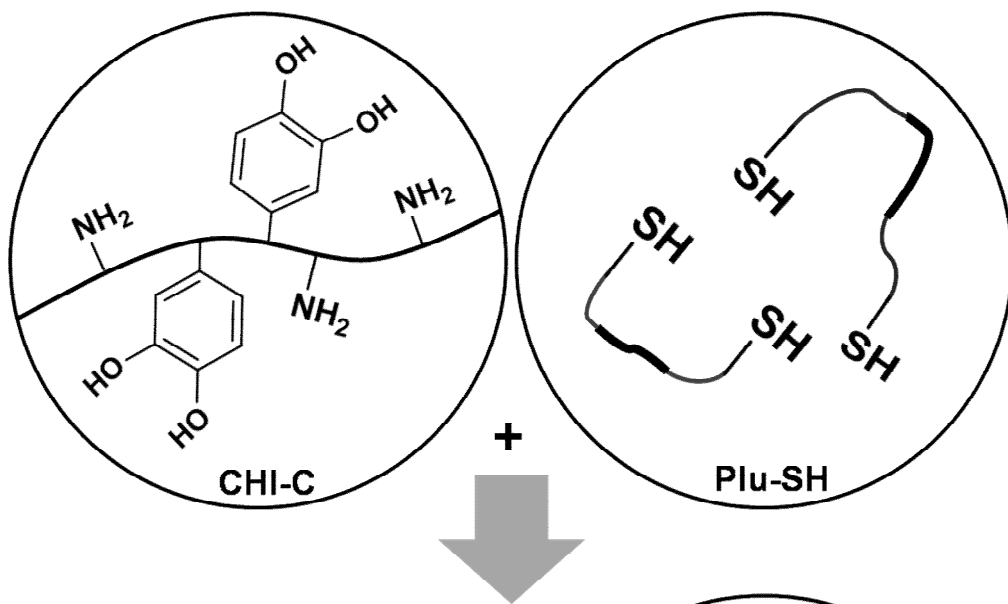
발표종류: 포스터, 발표일시: 목 15:00~17:00

Catechol Functionalized Chitosan/Pluronic Hydrogels for Tissue Adhesives and Hemostatic Materials

유지현, *채경민, *박태관

KAIST 나노과학기술대학원 *KAIST 생명과학과

Bio-inspired from adhesion behaviors of mussels, injectable and thermo-sensitive chitosan/Pluronic composite hydrogels were synthesized for tissue adhesives and hemostatic materials. In highly cross-linked mussel adhesive pad, catechol moiety (ortho-dihydroxyphenyl group) in unusual amino acid DOPA (3,4-dihydroxyphenylalanine) plays an important role in adhesion on various substrates and chemical bonding with amine, thiol, and other catechols. Chitosan conjugated with multiple catechol groups in the backbone was cross-linked with terminally thiolated Pluronic F-127 tri-block copolymer to produce temperature-sensitive and adhesive sol-gel transition hydrogels. A blend mixture of the catechol conjugated chitosan and the thiolated Pluronic F-127 was a viscous solution state at room temperature, but became a cross-linked gel state with instantaneous solidification at the body temperature and physiological pH. The adhesive chitosan/Pluronic injectable hydrogels with remnant catechol groups showed strong adhesiveness to soft tissues and mucous layers. The hydrogel systems also showed superior hemostatic properties possibly because of 1) strong hemostatic ability of chitosan molecules, 2) tissue adhesion of catechols, and 3) physical entrapment of wound site by rapid gelation. These novel chitosan/Pluronic hydrogels are expected to be usefully exploited for injectable drug delivery depots, tissue engineering hydrogels, tissue adhesives, and anti-bleeding materials.



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발표코드: II-POLY.P-36

발표분야: 고분자화학

발표종류: 포스터, 발표일시: 목 15:00~17:00

Transfer Printing of Micropatterned Polyelectrolyte Multilayer Films Prepared by a Spin Self-Assembled Method

이성근, 천세연, 강훈구, 노재근

한양대 화학과

Multilayered films prepared by layer-by-layer (LbL) assembly are promising candidates for a wide variety of applications such as electronic and optical devices, superhydrophobic surfaces, and biochemical sensors. Polyelectrolyte multilayers (PEMs) composed of Poly(ethyleneimine) (PEI)[poly(allylamine hydrochloride) (PAH)/ poly(sodium 4-styrenesulfonate) (PSS)]_n were grown as a function of dip and spin cycle of (PSS/PAH) bilayers. UV absorbance at 226 nm corresponding to PSS was proportionally increased with increasing the number of bilayers. AFM study revealed that surface morphology was changed before and after surface modification using PEMs. A PDMS was patterned with a master using conventional photolithography, and micropatterned PAH/PSS PEM films were successfully prepared onto the PDMS surface using dip or spin self-assembly (SA) methods. The micropatterned PAH/PSS PEM films were directly transferred to silicon surface with a sharp edge structure, which were conformed by atomic force microscopy measurements.

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장소: 제주ICC

발표코드: II-POLY.P-37

발표분야: 고분자화학

발표종류: 포스터, 발표일시: 목 15:00~17:00

Temperature Cycling Effects of Solvent Vapor Annealing in Thick Films by using Block Copolymer Micelles

김성남, 김승빈

포항공과대 화학과

We report that temperature cycling effect of solvent annealing in thick films by using block copolymer micelles. For this purpose, multilayered spherical micelles of poly(4-vinylpyridine) were prepared by spin-coating of polystyrene-block-poly(4-vinylpyridine) copolymer (PS-b-P4VP) in toluene/methanol mixture solutions on a silicon wafer with natural oxide layer. Very interestingly, when solvent vapor annealing was performed, these spherical micelles were transformed, via micelle fusion, into vertically oriented cylindrical microdomains spanning the entire film thickness up to several hundred nanometers because of solvent vapor pressure difference induced by controlling annealing temperature. It provides us the clue to understand solvent vapor annealing mechanism. Also, it would be simple method for the preparation of vertically oriented cylindrical microdomains in thick films by using block copolymer micelles and solvent vapor annealing. The effects of temperature cycling on the final morphology were investigated with scanning force microscopy and cross-section transmission electron microscopy. Vertically oriented cylindrical microdomains in a thick film could be employed for the templates for optical and optoelectronic applications.

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장소: 제주ICC

발표코드: II-POLY.P-38

발표분야: 고분자화학

발표종류: 포스터, 발표일시: 목 15:00~17:00

Synthesis and Characterization of poly (arylene ether sulfone) containing pendent quaternary ammonium groups for anion-exchange membrane fuel cell

이혜진, *김형준

서울대 화학생명공학부 *KIST 연료전지센터

Fuel cells are one of the alternative power sources in the future. The main advantage of AFC is possibility of use non noble metal catalyst such as Ag and improvement of water management. Nevertheless they also exhibit drawbacks due to use of liquid electrolyte such as KOH solution. Because hydroxide ion in electrolyte and carbon dioxide contained in air can form carbonates and liquid electrolyte may leak or flood on electrode, which affect efficiency and lifetime of AFC. In order to overcome these drawbacks, solid polymer electrolyte membrane was proposed. In this study, we present synthesis and characterization of poly (arylene ether sulfone) containing pendent quaternary ammonium groups for anion exchange membrane fuel cell. For ion conduction, 2-(2-(dimethylamino)ethyl)-3,3'-bis(4-hydroxyphenyl)isindolin-1-one (CPPH) group was introduced with different mole ratio and methylated to make quaternary ammonium groups. CPPH introduced copolymer showed relatively good conductivity and physical properties by different CPPH mol ratio. These results allow to possible candidates for AFC membrane.

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장소: 제주ICC

발표코드: II-POLY.P-39

발표분야: 고분자화학

발표종류: 포스터, 발표일시: 목 15:00~17:00

Nano-Patterning Process of Self-assembled Monolayer via Si-containing Block Copolymer Lithography on Gold Substrate

최수영, *김진백

KAIST 화학과 *KAIST 화학과

Chemical surface nanostructures were obtained using self-assembled monolayer patterned by microcontact printing or nanoimprint technique. But these approaches are inadequate at the micron- and sub-micron scales. Serial techniques like dip-pen and electron-beam lithographies achieve nanoscale pattern definition but are limited in their ability to define large area patterns. In this study, we use Si-containing block copolymer lithography for fabricating highly ordered nanoporous SiO₂ structures on gold substrates. The materials with silanol end groups self-assembled on the SiO₂ surface, while the compounds with the thiol groups on the gold surface. This dually patterned self-assembly method not only form ordered nanostructures over large area, but also offer dense periodic arrays of semiconducting inorganic oxide.

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장소: 제주ICC

발표코드: II-POLY.P-40

발표분야: 고분자화학

발표종류: 포스터, 발표일시: 목 15:00~17:00

Synthesis and Micellization of Amphiphilic diblock copolymers having Azobenzene as a side group by ATRP

장아름, *이창욱, **김지현, ***이승우

영남대 화학공학과 *영남대 응용화학공학과 **영남대 응용화학공학부 ***영남대 디스플레이화학공학부

Atom transfer radical polymerization (ATRP) has opened a new route to synthesize functional and architectural polymers with well-defined structures. In this work, poly(ethylene oxide)-b-poly(2-hydroxyethyl methacrylate) (PEO-b-PHEMA) was synthesized by successive ATRP of 2-hydroxyethyl methacrylate (HEMA) monomer using PEO-Br macroinitiator as an initiator, CuBr and 2,2'-bipyridyl (bpy) as a catalyst and a ligand, respectively. Poly(ethylene oxide) (PEO) and poly(2-hydroxyethyl methacrylate) (PHEMA) are two of the most frequently investigated classes of hydrophilic polymers. Then, amphiphilic diblock copolymers were prepared by the reaction of PEO-b-PHEMA, 4-phenylazobenzoic acid and 1-Ethyl-3-(3-dimethylaminopropyl)carbodiimide hydrochloride, 4-(Dimethylamino)pyridine. In this study, we prepared spherical micellar structure using the synthesized amphiphilic diblock copolymers. The formation of micellar structures was confirmed by a fluorescence technique by using pyrene as a probe. We were able to get a result of Azobenzene-containing diblock copolymer micelles undergo trans-cis isomerization on photo-irradiation. The trans isomer could be converted to the cis form by irradiating UV light of 360nm and the reverse transformation is achieved on the irradiation of 430nm light.

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장소: 제주ICC

발표코드: II-POLY.P-41

발표분야: 고분자화학

발표종류: 포스터, 발표일시: 목 15:00~17:00

A New Low Band Gap Conducting Polymer; Synthesis, Characterization and Property

박은랑, 정연준, 김인태

광운대 화학과

A new low band gap conducting polymer was successfully synthesized from a new compound as monomer by electrochemical polymerization. The electrochemically prepared polymer showed absorption maximum at 775nm in the UV-vis spectrum. The polymer was soluble in organic solvents, such as CHCl_3 , CH_2Cl_2 and THF. The characterization of the polymer includes $^1\text{H-NMR}$, $^{13}\text{C-NMR}$ and IR.

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장소: 제주ICC

발표코드: II-POLY.P-42

발표분야: 고분자화학

발표종류: 포스터, 발표일시: 목 15:00~17:00

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

황선우, 김홍선, 이상우, 김인태

광운대 화학과

A new conjugated polymer containing thiophene derivative was successfully synthesized by Stille's coupling reaction. The new polymer has good solubility in organic solvents such as CHCl_3 , DMF and Chlorobenzene. The new polymer was characterized by ^1H NMR, ^{13}C NMR, GPC and TGA. Electrochemical and optical properties of the polymer were measured by UV-vis spectroscopy, PL spectroscopy and cyclovoltammetry. The new polymer will be used for polymer solar cell device.

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장소: 제주ICC

발표코드: II-POLY.P-43

발표분야: 고분자화학

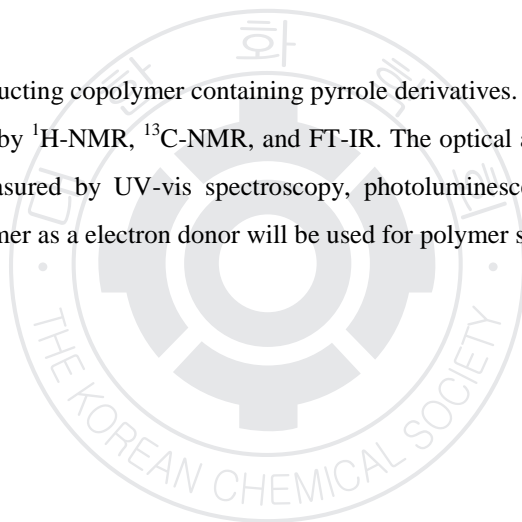
발표종류: 포스터, 발표일시: 목 15:00~17:00

Synthesis and Properties of a New Conducting Polymer

정연준, 김인태

광운대 화학과

We synthesized a new conducting copolymer containing pyrrole derivatives. The structure of the resulting polymer was characterized by $^1\text{H-NMR}$, $^{13}\text{C-NMR}$, and FT-IR. The optical and electronical properties of the new polymer was measured by UV-vis spectroscopy, photoluminescence and cyclovoltammetry, respectively. The new polymer as a electron donor will be used for polymer solar cells.



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장소: 제주ICC

발표코드: II-POLY.P-44

발표분야: 고분자화학

발표종류: 포스터, 발표일시: 목 15:00~17:00

Synthesis of Polyelectrolyte Complex Particles with Reversible Structure as a Chemical Nanoreactor: An Ideal Nanocatalyst for Devouring Poisons

Md. Shahinul Islam, *최원산, *이하진, 전일철

전북대 화학과 *한국기초과학지원연구원 전주센터

The spherical polyelectrolyte complexes (nPEC) were synthesized by adjusting the mixing ratio of two kinds of weak polyelectrolytes such as poly(allylamine hydrochloride) (PAH) and poly(acrylic acid) (PAA), without using any sacrificial template. After loading of Au and Ag precursors on the nPEC, Au, Ag as well as Au-Ag alloy nanoparticles (NPs) were synthesized by thermal reduction. The structure of the resulting metal NPs-embedded nPEC particles could be reversibly tuned by varying a pH condition. They were swelled and restored to original size in a range from 200 nm to 800 nm. This means that distribution and density of metal NPs within the nPEC particles can be easily controlled upon structural change of nPEC particles. As a result, close packing or loose packing structure of NPs was formed within the shrunk or swelled nPEC particles, respectively. The resulting Au-Ag alloy NPs-embedded nPEC showed excellent catalytic performance for the reduction of 4-nitrophenol which is considered as toxic materials, compared with Au NPs.

일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: II-POLY.P-45

발표분야: 고분자화학

발표종류: 포스터, 발표일시: 목 15:00~17:00

Photoinitiation in RAFT process of vinyl acetate

함민경, 곽영제

충청대 유기신소재파이버공학과

Radical addition and fragmentation chain transfer (RAFT) process is one of the controlled radical polymerization techniques that prepare polymers with pre-determined molecular weight and low polydispersity. However controlling stereoregularity is not easy because of the intrinsic nature of the active radical species which are of low energy barrier between two enantiomers. To improve stereoregularity of the prepared polymer, lowering polymerization temperature is generally preferred. In this work, we used photoinitiation process to generate radicals in RAFT of vinyl acetate. We studied photochemical properties of RAFT agents. It's because photolysis of these functional groups diminishes overall polymerization control, causing an increase in polydispersity index. To suppress this undesired photolysis we used filter to modulate the range of effective UV source. With careful selection of photoinitiator, UV radiation wavelength, intensity and structure of RAFT agent, it was possible to prepare polymers with controlled architectures.

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발표코드: II-POLY.P-46

발표분야: 고분자화학

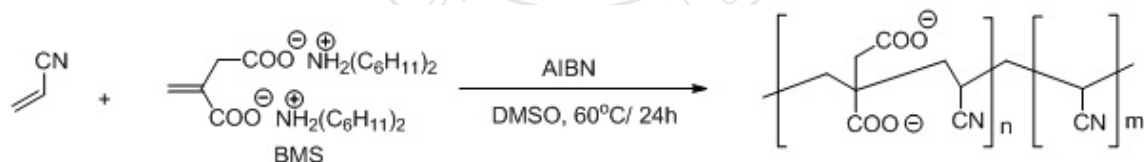
발표종류: 포스터, 발표일시: 목 15:00~17:00

Synthesis and Thermal Behavior of Carbon Fiber Precursor from Acrylonitrile and Bis(dicyclohexylammonium)-2-methylenesuccinate as a Comonomer.

신동근, 기세훈, 한진욱, *김기영

한양대 화학과 *한국생산기술연구원 섬유융합연구그룹

Carbon-fiber has been paid attention in a broad range of application, such as aerospace, automobile, and sport goods. High performance carbon-fiber precursors from new comonomers have been developed. This study used bis(dicyclohexylammonium)-2-methylenesuccinate (BMS) as a new comonomer in PAN polymerization. It was revealed that thermal properties changed by the content of BMS in PAN polymerization.



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발표분야: 고분자화학

발표종류: 포스터, 발표일시: 목 15:00~17:00

Fabrication of Nanoporous Templates with High Aspect Ratio Using Silicon-Containing Block Copolymers and Dual Responsive Bilayer Systems

박창홍, 조경천, 김진백

KAIST 화학과

A simple and scalable method was developed to fabricate a nanoporous template for freestanding one-dimensional nanostructure arrays based on self-assembly of silicon-containing block copolymers and a lithographic bilayer system. Removal of the cross-linked bottom layer after fabrication is not easy. Therefore, we propose a dual responsive bottom layer into which the nanopatterns of block copolymer are transferred by oxygen reactive ion etching. Because the dual responsive layer becomes cross-linked by heating, it can be used as a hard template during the etching process. It becomes soluble again by chain scission upon exposure to light. Therefore, it can be easily removed by the lift-off process. The results will be described in detail.

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발표코드: II-POLY.P-48

발표분야: 고분자화학

발표종류: 포스터, 발표일시: 목 15:00~17:00

Synthesis and Properties of Covalently Cross-linked Polyimide

권세진, *이상현, 서혜미, **이승우

영남대 화학공학과 *영남대 화공과 **영남대 디스플레이화학공학부

We describe polyimide films for flexible display substrate which should have high heating resistance and low CTE (coefficient of thermal expansion) values. A series of polyimide containing were synthesized by conventional solution polymerization. Thermally cross-linked moieties were prepared by the reaction of 4-Phenylethynylphthalic anhydride (4-PEPA), 2,2'-Bis-(3,4-Dicarboxyphenyl) hexafluoropropane dianhydride (6FDA), 2,2'-Bis(trifluoromethyl)benzidine (22TFMB) in N,N-dimethylacetamide (DMAc). The molecular structures of the composite materials were investigated and ¹H-NMR by means of Fourier transform infrared spectrometer (FT-IR). Thermogravimetric analysis (TGA), Differential scanning calorimetry (DSC) and Dynamic mechanical thermal analysis (DMTA) showed that the excellent thermal stability of polyimides.

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발표코드: II-POLY.P-49

발표분야: 고분자화학

발표종류: 포스터, 발표일시: 목 15:00~17:00

Conductive polymer photopatterning on photo cross-linkable EDOT having azide pendant group and its electrochromic diffraction switching application

YANGXU, *김유나, *김은경

연세대 화공생명공학과 *연세대 화학공학과

Photo-patternable conductive polymer, poly(2-(azidomethyl)-2,3-dihydrothieno[3,4-b][1,4]dioxine) (PEDOT-MZ) was prepared via vapor phase polymerization, from EDOT-MZ monomer. Micro sized patterns were generated by simple UV exposure onto the films through a photomask and observed by microscopy. The photo-cross linking from the azide side chain was confirmed by FT-IR and AFM, which showed surface morphologies change due to the photo reaction. The optical and electrochemical properties were measured by UV-vis absorbance and cyclic voltammetry respectively. After UV exposure, the conductivity of PEDOT-MZ film decreased about 800 times and the electrochromic (EC) efficiency decreased 50 % compared to the pristine film. The photo patterned PEDOT-MZ film was prepared to EC cell by simple method and showed switchable electrochromism and diffraction properties, that can be easily applied in organic electrodes, electrochromic devices, electrochemical light-emitting, and solar cells.

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발표코드: II-POLY.P-50

발표분야: 고분자화학

발표종류: 포스터, 발표일시: 목 15:00~17:00

Synthesis and Characterization of New Liquid Crystalline Diblock Azo Copolymers via RAFT Polymerization and Their Morphology

ZENATIATHMEN, 이제권, 한양규

한양대 화학과

Liquid crystals (LCs) are very important in the study of optics, chemistry, and polymer science. A novel photoresponsive monomer (SCAM) with silicon-containing azobenzene moiety in the side chain was synthesized by reacting 3-acryloxypropylmethyldichlorosilane with 2-[2-(4-cyano-azobenzene-4'-oxy)ethylene-oxy]ethyl alcohol, a mesogenic unit. Corresponding well-defined azobenzene-containing diblock copolymers, Poly(SCAM-b-MMA), were prepared via reversible addition fragmentation chain transfer (RAFT) polymerization in THF solution with PMMA macro-RAFT-agent and SCAM in the presence of AIBN. The structures and properties of the monomer and the diblock copolymers were characterized by ¹H NMR, DSC, IR, and GPC, respectively. In addition, their liquid crystallinity and morphological structure were observed by optical polarizing microscopy and AFM.

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장소: 제주ICC

발표코드: II-POLY.P-51

발표분야: 고분자화학

발표종류: 포스터, 발표일시: 목 15:00~17:00

Stabilization of Cysteine-Covered Dendron-Cyclodextrin Nanotubes

이정훈, 김철희

인하대 고분자공학과

본 연구팀에서는 focal point 에 pyrene 을 도입한 amphiphilic amide dendron 이 수용액상에서 vesicle 형태로 self-assembly 되었다가 β -cyclodextrin(β -CD)과 inclusion complex 를 형성하게 함으로써 표면이 β -CD 로 덮여진 나노튜브로 self-assembly 되는 현상을 규명한 바 있다. 또한 나노튜브 표면에 있는 CD 의 C6 위치의 -OH 그룹을 원하는 다양한 작용기로 치환하여 다양한 기능을 갖는 나노튜브를 만들 수 있다는 것도 규명하였다. 본 연구에서는 다양한 용매조건에서 자기조립된 나노튜브의 stability 를 향상시키키위하여 CD 의 작용기를 cysteine moiety 로 치환하여 나노튜브의 표면에 cysteine 을 도입하였다. 그 후, 표면의 thiol 기를 이용하여 튜브의 표면을 crosslinking 시키는데 성공하였고, 이를 통해 covalent bond 로 연결된 표면을 갖는 나노튜브를 제조하였으며, 이를 TEM, SEM 등으로 확인하였다. 또한, 이렇게 만들어진 self-assembled structure 의 stimuli-responsive transformation 현상도 관찰하였다.

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발표코드: II-POLY.P-52

발표분야: 고분자화학

발표종류: 포스터, 발표일시: 목 15:00~17:00

Polymeric Vesicles with a Hydrophobic Interior Formed by Thiophene-Based All-Conjugated Amphiphilic Diblock Copolymer

임민정, 문병준, 박태호

포항공과대 화학공학과

Over the last several decades, coil-coil or rod-coil diblock amphiphiles have been extensively studied for their ability to form well-defined self-assembled vesicles for use in drug and gene delivery, among other applications. Their applications may now be extended to photonics and biosensors due to the development of amphiphilic rod-rod block copolymers composed of dielectric-conjugated blocks or all-conjugated blocks. Recently, McCullough et al. and Yokozawa et al. developed a novel one-pot synthetic method for preparing regioregular aromatic polymers via Grignard metathesis (GRIM). Using this method, Tajima et al. and others independently reported the successful synthesis of thiophene-based all-conjugated diblock copolymers. Here, we report the formation of an unusual p-p stacking-driven polymeric vesicles a few hundred nm in scale from thiophene-based all-conjugated amphiphilic diblock copolymer.

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발표분야: 고분자화학

발표종류: 포스터, 발표일시: 목 15:00~17:00

Thiophene-Based All Conjugated Diblock Copolymers

문병준, 임민정, 박태호

포항공과대 화학공학과

Up to now, preparations of rod-rod block copolymers have been mainly prepared from macro-initiators to introduce a second block, but this technique has resulted in low reaction yields, low molecular weight products, or difficulties in isolating the products. Recently, McCullough et al. and Yokozawa et al. developed a novel one-pot synthetic method for preparing regioregular aromatic polymers via Grignard metathesis (GRIM). Using this method, Tajima et al. and others independently reported the successful synthesis of thiophene-based all-conjugated diblock copolymers. Here, we reports thiophene-based all conjugated diblock copolymers synthesized by the quasi-living polymerization. These block copolymers permit access to a range of morphologies depending on the fractions of components. We observed the self-assembly phenomena and its properties.

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발표코드: II-POLY.P-54

발표분야: 고분자화학

발표종류: 포스터, 발표일시: 목 15:00~17:00

Intramolecular charge transfer complexation in D-A types of conducting polymers

이강영, 박태호

포항공과대 화학공학과

Much interest is in conjugated copolymers consisting of donor and acceptor units due to application in organic photovoltaic devices. Intramolecular CT complexes may be formed using materials with alternating electron-rich carbazole derivatives (electron donor: D) and electron-deficient moieties (electron acceptor: A). Depending upon structures of the copolymer such as types of donor and acceptors, side chains, and dihedral angles, ability of intramolecular charge complexation might be different, dominating the electrochemical, optical, and electronic properties of the resulting polymers. Here, we report that synthesis of novel D-A types of conducting polymers. Especially, we investigated parameters influencing optoelectronic properties which are controlled by conjugation length and steric hindrance.

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장소: 제주ICC

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발표분야: 고분자화학

발표종류: 포스터, 발표일시: 목 15:00~17:00

Cell-penetrating Peptide-decorated Human Serum Albumin/PEG shell cross-linked Nanocapsules for Efficient Delivery of Paclitaxel

이정유, 배기현, 김지선, *김규리, 박태관

KAIST 생명과학과 *KAIST 나노과학기술대학원

To develop hydrophobic drug delivery efficiency, paclitaxel-encapsulating human serum albumin nanocapsules (PTX/HSA nanocapsules) were produced by cross-linking of albumin with N-hydroxysuccinimide-functionalized 6-arm branched poly (ethylene glycol) at the organic/aqueous interface. These PTX/HSA nanocapsules had a spherical shape with an average diameter of about 270-300nm and were well dispersed and separated from each other, indicating that the cross-linked capsule framework prevented the encapsulated paclitaxel from aggregating into crystal form. The encapsulation efficiency was about 47-74% of the paclitaxel encapsulated at a weight ratio of 9-14% (w/w). As efficient paclitaxel carrier, the albumin nanocapsules showed superior induction cancer cell death compared with TAXOL. Confocal microscopy revealed that Hph 1-conjugated HSA nanocapsules significantly enhanced the cellular uptake and apoptotic effect against cancer cells. Furthermore, paclitaxel-encapsulating albumin nanocapsules show great potential through in vivo tests with the high level of drug delivery efficiencies, even in the absence of targeting system. The present study suggested that paclitaxel-encapsulating albumin nanocapsules have a future as potential candidates for efficient drug delivery system.

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발표코드: II-POLY.P-56

발표분야: 고분자화학

발표종류: 포스터, 발표일시: 목 15:00~17:00

Synthesis and Characterization of Fluorene and Cyclopentadithiophene-based Copolymers Exhibiting Broad Absorption for Photovoltaic Devices

정인환, 심홍구

KAIST 화학과

We have synthesized two low band gap copolymers composed of fluorene (Fl), cyclopentadithiophene (CDT) and 4,7-bis(2-thienyl)-2,1,3-benzothiadiazole (DBT), and their optical, electrochemical and photovoltaic characteristics were investigated for applications in photovoltaic devices. The feed ratio of the Fl and CDT moieties was modulated to tune the electronic structures and resulting optical properties of the polymers. In the copolymeric structures, the Fl-CDT unit absorbs the short-wavelength UV/vis regions and the CDT-DBT (or Fl-DBT) unit with strong intramolecular charge transfer characteristics covers the long-wavelength visible regions. P1 exhibited a wide UV absorption spectrum covering the UV and entire visible region in the range of 300 nm ~ 800 nm, and P2 showed absorption covering from 300 nm to 700 nm. UV/vis and electrochemical studies confirmed the desirable HOMO/LUMO levels of the copolymers with band gaps of 1.62 ~ 1.86 eV, enabling efficient electron transfer and a high open circuit voltage when blending them with fullerene derivatives. When the polymers were blended with [6,6]phenyl-C61-butyric acid methyl ester (PCBM), P1 exhibited the best device performance with an open circuit voltage of 0.66 V, short-circuit current of 4.92 mA/cm² and power conversion efficiency of 1.13 % under air mass 1.5 global (AM 1.5G, 100 mW/cm²) illumination.

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발표분야: 고분자화학

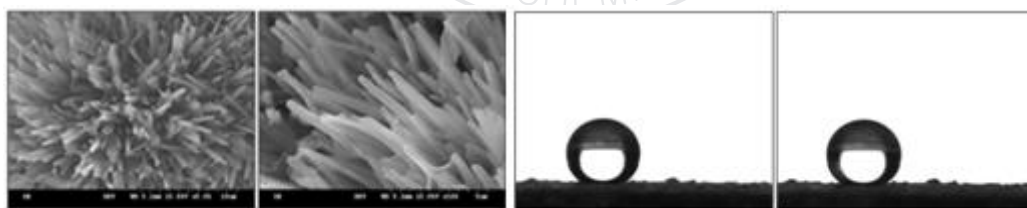
발표종류: 포스터, 발표일시: 목 15:00~17:00

Facile fabrication of polysiloxane nanorods on magnesium surface in the presence of 1,6-diphosphono-hexane

고승철, 박연화, 안용현

단국대 화학과

Polysiloxane nano-rods was prepared by coating Mg substrates with a mixture solution of alkyl triethoxysilane and 1,6-diphosphono-hexane in ethanol. The morphology control of nano-rods on Mg surface was obtained using the 1,6-diphosphono-hexane. The resulting substrates were characterized by scanning electron microscopy, contact angle measurements, X-ray photon electron spectroscopy and external Fourier transform infrared spectroscopy. This paper showed the fabrication of very high crystalline polysiloxane nano-rods from silane derivatives in the presence of 1,6-diphosphono-hexane. Phosphate derivative functions as a structure modifier.



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발표분야: 고분자화학

발표종류: 포스터, 발표일시: 목 15:00~17:00

Syntheses, Characterization and Substituent Effect of New Blue or White Emitters based on Naphthalene Core for OLEDs

김동원, *박종욱, **정민철, 이지훈

충주대 나노고분자공학과 *가톨릭대 화학과 **순천대 화학공학과

π -conjugated organic materials 의 전자산업으로의 응용은 최근 Organic light-emitting diodes (OLEDs)를 이용한 디스플레이 분야에서 그 유용함이 크게 두드러지게 나타나고 있다. 이러한 OLED 의 급속한 발전으로 인해 현재는 Organic Light Emitting Diode(OLED)가 Liquid crystal Display(LCD)를 위협하는 가장 강력한 디스플레이 경쟁자로 주목받고 있다. 특히, 백색을 이용한 WOLED 기술은 디스플레이 뿐만아니라 기존의 백열등, 형광등을 대신할 조명으로서 상당한 중요성을 가지고 있다. 특히나 모든 색을 구현하는 디스플레이에서 R, G, B 삼색은 모두 똑같은 중요도를 갖지만, 백색발광은 원하는 모든 색을 필터링을 통해 구현할 수 있기 때문에, 크게 주목 받는다. 이에 우리는 Single molecule 수준에서 white emission 을 나타내는 새로운 재료를 개발하는데 중점을 두었다. 합성된 재료는 naphthalene core 에 입체적으로 bulky 한 9,10-diphenylanthracene side groups 들을 도입하였으며 naphthalene 2,6 위치와 1,4 위치에 9,10-diphenylanthracene 을 도입한 새로운 single molecule 5 종을 합성하여 분자의 특성 변화를 연구하였다. 합성 방법은 n-BuLi 을 통한 lithiation 방법과 Pd(0) catalyst 를 이용한 Suzuki aryl-aryl coupling reaction 을 통해 최종 목적 화합물을 합성하였다. 합성된 재료는 NMR, IR 등의 분광학적 방법으로 분석하였으며 재료의 광학적, 열적, 전기화학적 특성 등을 조사하였다.

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발표코드: II-POLY.P-59

발표분야: 고분자화학

발표종류: 포스터, 발표일시: 목 15:00~17:00

Highly Selective Reduction of Aromatic Nitro Compounds Using a New Polymer Reagent

전보람, 김수화, 한양규

한양대 화학과

We synthesized a new porous crosslinked copolymer particle from styrene and new monomer in the presence of divinyl benzene by a suspension polymerization(DS28D). The porous polymer was used as a polymer reagent for conventional organic reductions: nitrobenzene and its derivatives(o-ethyl nitrobenzene, o-methyl nitrobenzene and so on) were reduced in high yield by using a Zn/NH₄Cl system in water in the presence of the prepared copolymer particles without any organic solvent at mild conditions. Unlike the conventional reduction utilizing the Zn/NH₄Cl system, the use of small amount of polymer reagent enables the highly selective reduction of nitrobenzene derivatives to azoxybenzene compounds due to the orientation effects of the polymer reagent.

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발표분야: 고분자화학

발표종류: 포스터, 발표일시: 목 15:00~17:00

New Poly(arylene ether)s with Transparency and High Heat-resistance

권경재, 이원중, 변인준, 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 FBPODS, an ordered-sequence aromatic dihalide, and cardo typed aromatic diols that contain fluorene or adamantane moiety. The resulting polymers were found to be amorphous by X-ray diffractometry and T_g ranged from 200 to 250 °C. Based on TGA and TMA data, they exhibited excellent thermal stabilities. They had good mechanical properties with modulus of 1750-2150 MPa. The optical transmittance for the PAE films (ca. 20 μm thick) was over 70% at 450-800 nm and they also showed water uptake of about 0.65% regardless of their chemical composition.

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장소: 제주ICC

발표코드: II-POLY.P-61

발표분야: 고분자화학

발표종류: 포스터, 발표일시: 목 15:00~17:00

Fabrication of High Aspect Ratio Nanoporous Templates Using Silicon-Containing Block Copolymers and One-dimensional(1D) Nanostructure.

조경천, 김진백, 박창홍

KAIST 화학과

Well defined nanoporous templates with high aspect ratios are highly desirable for a variety of applications. In this study, we combined bilayer approach with block copolymer lithography. This system consists of a top silicon-containing block copolymer layer and an underlying SU-8 layer into which the nanopatterns of block copolymers are transferred by oxygen reactive ion etching. This nanoporous template can be applied to the fabrication of nanorods and nanotubes using electrodeposition and atomic layer deposition. The results will be described in detail.

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장소: 제주ICC

발표코드: II-POLY.P-62

발표분야: 고분자화학

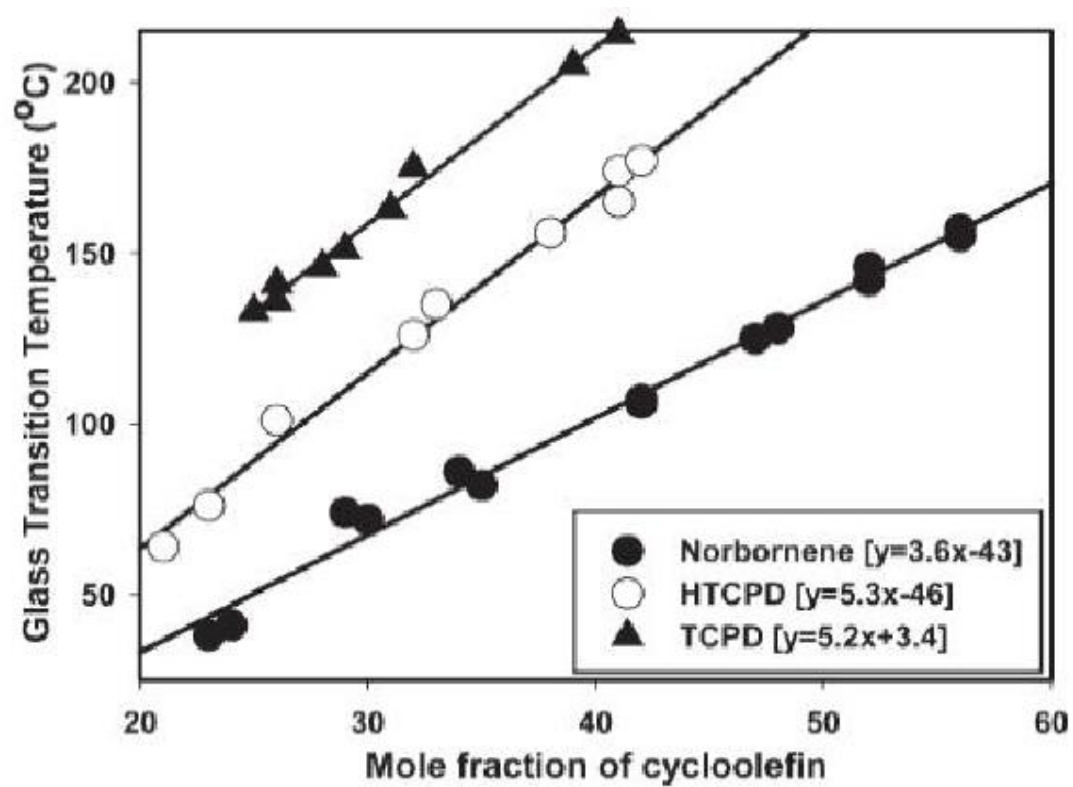
발표종류: 포스터, 발표일시: 목 15:00~17:00

Preparation of Cycloolefin Copolymers of a Bulky Tricyclopentadiene

오경환, 김아름, 이분열

아주대 분자과학기술학과

Regioselective partial hydrogenation of tricyclopentadiene (TCPD) was achieved with a high TON (turnover number) of 10000 by employing an N-heterocyclic carbene palladium complex as a catalyst. Copolymerization of ethylene and the partially hydrogenated product, dihydrotricyclopentadiene (HTCPD), was realized using a catalytic system of $[8-(\eta^5-C_5Me_4)-2-Me(C_9H_8N)-\kappa N]TiMe_2$ ($C_9H_{10}NH = 1,2,3,4$ -tetrahydroquinoline) activated with $(Ph_3C)^+[B(C_6F_5)_4]^-$. And copolymerizations of ethylene and tricyclopentadiene (TCPD) are realized without cross-linking with a high activity ($3 - 18 \times 10^6$ g/molZr·h) using a catalytic system of $[Ph_2C(Flu)(Cp)]ZrCl_2/MAO$. These polymer has high Tg, ethylene/HTCPD copolymer Tg is 177°C, ethylene/TCPD copolymer is 214°C. This is significantly higher than that of norbornene/ethylene copolymer at the same cycloolefin content.



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발표분야: 고분자화학

발표종류: 포스터, 발표일시: 목 15:00~17:00

Glutathione-Responsive Silica-Iron Nanocontainers with Cyclodextrin Gatekeepers for Acting simultaneously in Delivery and Imaging

김현정, 이정훈, 김철희

인하대 고분자공학과

본 연구에서는 core 에 자기공명영상을 위한 조영제로 사용되는 iron oxide(직경 22 nm)를 가지는 MCM-41 타입 실리카 나노입자(Fe@SiNP , 직경 60 nm, pore 2 nm)의 pore 입구에 gatekeeper 를 장착하여, pore 내부에 봉입된 약물을 특정한 외부 자극을 가하여 방출시킬 수 있는 새로운 방법을 확립하였다. Fe@SiNP 의 표면에 gatekeeper 인 cyclodextrin (CD)을 disulfide bond 를 통해 도입하였다. 본 시스템에서는 GSH 가 없는 조건에서 장시간 동안 약물의 방출이 억제되며, GSH 가 있는 조건에서는 gatekeeper 와 Fe@SiNP 를 연결하는 disulfide bond 가 thiol 로 환원되어 CD 가 Fe@SiNP 로부터 제거되면서 약물을 방출시킨다. Fe@SiNP 의 구조와 특성은 FT-IR, BET, TEM, SEM, PL, CLSM 등으로 규명하였다. 또한, in vitro 와 in vivo 실험을 통하여 Fe@SiNP 의 약물전달체로서의 특성을 규명하였고, MRI 를 통해 Fe@SiNP 가 조영제로써의 역할도 함께 수행할 수 있으며, EPR effect 로 암세포를 진단할 수 있음을 밝혔다.

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발표분야: 고분자화학

발표종류: 포스터, 발표일시: 목 15:00~17:00

Fabrication of TiO₂ nanostructures enabled by block copolymer template-assisted method and their application in dye-sensitized solar cells

장윤희, *Xukai Xin, *Myunghwan Byun, *Zhiquan Lin, 김동하

이화여대 화학나노과학과 *Department of Materials Science and Engineering, Iowa State University

The dye-sensitized solar cells (DSSCs), which are one of the most important photovoltaic devices, have been become a promising candidate for the future renewable energy production due to their high solar energy conversion efficiency and relatively low fabrication cost. Various types of TiO₂ nanostructures, including mesoporous nanocrystalline films, nanotubes, nanorods, and nanowires, have been reported and yielded the high power conversion efficiency. Herein, two-dimensional arrays of TiO₂ nanostructures including nanodots or nanorings were fabricated by a synergetic process of self-assembly of PS-*b*-P4VP diblock copolymer and sol-gel reaction. Their potential uses as photoanodes for DSSCs were experimentally investigated: TiO₂ nanostructures were directly fabricated on fluorine-doped tin oxide glass and then N719 ruthenium sensitizer and ionic liquid electrolyte were employed.

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장소: 제주ICC

발표코드: II-POLY.P-65

발표분야: 고분자화학

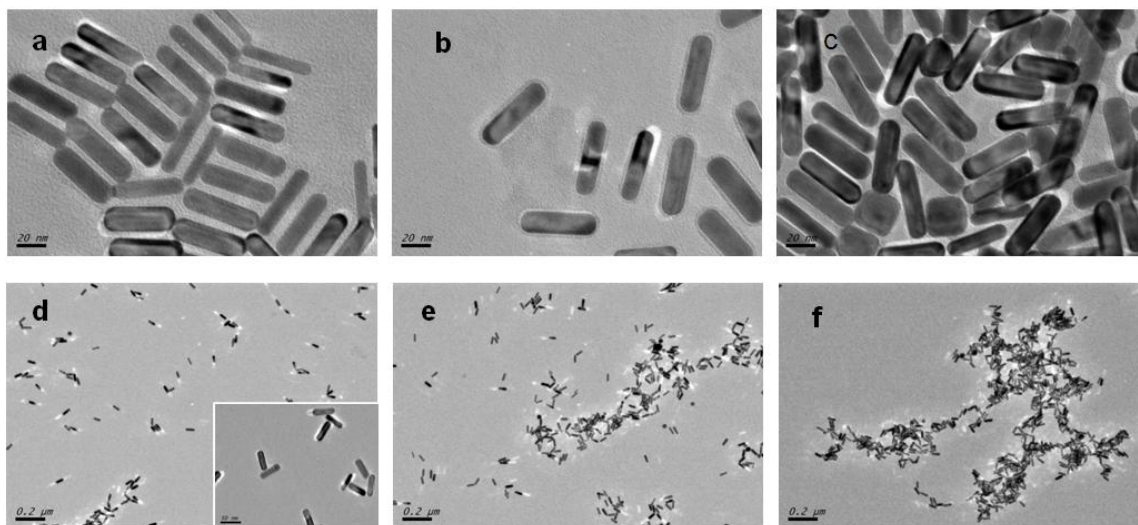
발표종류: 포스터, 발표일시: 목 15:00~17:00

pH-Responsive Nanostructures of Poly(4-vinylpyridine)/Gold Nanorods

Dongxiang Li, *김동하

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Poly(4-vinylpyridine) grafted gold nanorods (Au NRs) were synthesized by a surface-initiated atom-transfer radical polymerization (SI ATRP). Herein, we found that the immobilization of disulfide initiator to the nanorod surface was a key step because the CTAB-protected AuNRs (Fig. 1a) were easily aggregated in the disulfide exchange, so poly(ethyl glycol) (PEG) thiol was used as a mediate ligand to generate well dispersed PEG-protected AuNRs (Fig. 1b) and then the disulfide initiator was immobilized on the nanorod surface (Fig. 1c) for SI ATRP reaction in DMF. After the polymerization of 4-vinylpyridine, the obtained poly(4-vinylpyridine)/AuNR nanostructures (AuNR@PVP) was monodispersed at low pH but showed responsive assembly behaviors as pH increases from pH 2.03 (Fig. 1d), pH 3.39 (Fig. 1e) and pH 5.6 (Fig. 1f).



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발표분야: 고분자화학

발표종류: 포스터, 발표일시: 목 15:00~17:00

Growth of Polymer Brushes on Polyimide Films Surface by Surface-Initiated Atom Transfer Radical Polymerization

길은경, *장아름, **이창욱, ***이승우

영남대 화학공학 *영남대 화학공학과 **영남대 응용화학공학과 ***영남대 디스플레이화학공학
부

In recent years there has been increasing interest in surface-initiated polymerization reactions because they allow to modify and control the surface properties of materials to a high extent. In this study, We modified polyimide films surface using Atom Transfer Radical Polymerization(ATRP). In here, in order to immobilize initiator for ATRP, we applied micro-contact printing(M-CP) on polyimide films. Then, surface of the PI film was functionalized with 2-bromo-2-methyl propionic acid and the graft polymerization of methyl methacrylate(MMA) was carried out using the CuBr/bpy system for ATRP.

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장소: 제주ICC

발표코드: II-POLY.P-67

발표분야: 고분자화학

발표종류: 포스터, 발표일시: 목 15:00~17:00

Copolymerization of CO₂, Propylene Oxide: Precise Control of Molecular Weight and Architecture of Various Block Copolymers by Various Chain Transfer Agent

이상환, Anish Cyriac, 이분열

아주대 분자과학기술학과

Recently, CO₂/epoxide copolymerization has drawn much attention in both academic and industrial fields. A highly active and relatively cheap catalyst for CO₂/propylene oxide (PO) copolymerization is developed (TOF 15000 h⁻¹). It was revealed that the high activity of these kind of complexes, due to an unusual binding mode of a Cobalt(III) complex prepared from a Salen-type ligand tethered by four quaternary ammonium salts. This catalyst preserves an excellent catalytic performance even in the presence of a large amount of protic compounds which enables us to efficiently perform "immortal polymerization" in CO₂/propylene oxide copolymerization. Precise control of molecular weight is achieved by feeding various protic compounds such as adipic acid, which resulted in the formation of low molecular weight poly(propylene carbonate)-diol (PPC-diol). Using PPC-diol, we have demonstrated polyurethane formation. Various three armed and star shaped polymeric structures made by simply feeding three armed and four armed carboxylic acids. By feeding bulk polymer contains OH or COOH in immortal polymerization, we have demonstrated block and graft copolymerization. Additional melting region with slightly higher glass transition temperature is introduced by feeding PE-monoalcohol or PEG. A sheet prepared from PPC-*block*-PEG of 8.3 w% PEG unit is not as brittle as that of PPC itself. It is flexible and stretchable as the conventional PE film. A sheet prepared from PPC-*block*-PS of 11 w% PS unit is translucent and tougher than PPC itself.

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장소: 제주ICC

발표코드: II-POLY.P-68

발표분야: 고분자화학

발표종류: 포스터, 발표일시: 목 15:00~17:00

Safe and Cultivate for The Cell from Thermo-Responsive Aqueous Gels

황철강, *조혜정, 이명수

서울대 화학과 *서울대 화학부

Aqueous nanofibers constructed by self-assembly of small amphiphilic molecules are able to entangle with each other to form hydrogels that have a variety of applications including tissue engineering, and controlled drug delivery. The hydrogels are formed through physical cross-links in a random way of flexible nanofibers. Here we report that the self-assembled nanofibers with a nematic substructure are aligned into a nematic liquid crystal and spontaneously fixed in the aligned state to give rise to anisotropic gels. The liquid crystal gels are responsive to temperature variation by transformation into a fluid solution on cooling. Thus, the nanofiber solution can be mixed with cells at room temperature and transformed into gels to encapsulate the cells in a 3D environment upon heating to physiological temperatures. We found that the cells grow within the 3D networks without compromising cell viability, and subsequent cooling triggers the encapsulated cells to be released through a sol-gel transition. We anticipate that our smart nematic gels offer novel opportunities in many biological applications including tissue regeneration and drug delivery vehicles.

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장소: 제주ICC

발표코드: II-POLY.P-69

발표분야: 고분자화학

발표종류: 포스터, 발표일시: 목 15:00~17:00

Manufacturing of Fragrant Microencapsulation by Complex Coacervation using Gelatin and Cellulose Derivatives

고은주, *정근우, **박수열

한국화학연구원 그린화학연구단 *한국화학연구원 응용화학연구단 **한국화학연구원 색소화학
연구팀

Microcapsules coming fragrant oil were prepared by complex coacervation of gelatin and acacia or C.M.C as well materials. The processing parameters such as concentration of encapsulants, wall materials ratio, oil concentration, content of hardening agent, dispersing speed have been investigated for optimization. The microcapsules formation mainly affected by the wall materials ratio and oil concentration. It was also found that the particle size of the microcapsules decreased with an increasing stirring rate in emulsification process. The shape if microcapsules was an irregular sphere and average diameter of the particles were in the range of 23 um to 90 um as evidenced by Scanning Electron Microscopy (SEM). The chemical structure and the thermal characteristics of the resultant microcapsules were identified with Fourier Transform Infrared Spectrophotometry (FT-IR), Thermogravimetry (TGA) and Differential Scanning Calorimetry (DSC). Susceptible cotton and silk fabrics with fragrant release functionality were successfully produced by using these microcapsules containing fragrant microcapsules.

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장소: 제주ICC

발표코드: II-POLY.P-70

발표분야: 고분자화학

발표종류: 포스터, 발표일시: 목 15:00~17:00

Three New 1-(2,6-Diisopropylphenyl)-2,5-di(2-thienyl)pyrrole Based Polymers for Bulk Heterojunction Solar Cell Applications

V. Tamilavan, *진성호, 현명호

부산대 화학과 *부산대 화학교육과

A broad absorbing random copolymer namely PTTPTB-P1 containing 3-octylthiophene, 1-(2,6-diisopropylphenyl)-2,5-di(2-thienyl)pyrrole and 2,1,3-benzothiadiazole was synthesized. The absorption and energy levels of the PTTPTB-P1 polymer was fine tuned by using different ratio of donor and acceptor units, yielding two new random copolymers namely PTTPTB-P2 and PTTPTB-P3. The copolymers were characterized by using conventional methods such as GPC, NMR and UV. The optical band gaps of the polymers estimated from the onset wavelength of the absorption were identical for all three polymers (~1.80 eV). The energy levels of the copolymers were found to be suitable for BHJ solar cells applications. Each of the polymers was investigated as an electron donor blending with PC70BM as an electron acceptor in bulk heterojunction (BHJ) solar cells. BHJ solar cells were fabricated in ITO/PEDOT:PSS/polymer:PC70BM (1:5 wt%)/TiO₂/Al configurations. The BHJ solar cell with PTTPTB-P1:PC70BM (1:5 wt %) showed the power conversion efficiency (PCE) of 1.42% (J_{sc} = 8.08 mA/cm², V_{oc} = 0.56 V, FF = 31%), measured using AM 1.5G solar simulator at 100 mW/cm² light illumination.

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발표분야: 고분자화학

발표종류: 포스터, 발표일시: 목 15:00~17:00

Cure Kinetics Control of Epoxy Resins for Stone Conservation (or Restoration) by Varying Hardener

최용석, *강용수

한양대 화학공학과 *한양대 에너지공학과

Epoxy resins are widely used to conserve (or restore) damaged stone cultural heritages. When epoxy resin is mixed with a hardener during stone treatment, curing reactions occur, resulting in generation of heat due to the exothermic reactions. The heat generated could damage the structure of damaged stones further depending on its amount. Therefore, the heat should be carefully managed to provide proper conservation process: The lower is the amount of the heat generation rate by decreasing the curing kinetics and the better while maintaining the degree of curing. Here, hydrogenated bisphenol A ST-3000 (HBA, Kukdo Co.), fast curing agent KFH-548 (Kukdo Co.) and Jaffamine D-230 were used. Cure kinetics of epoxy/amine hardener systems was investigated using an isothermal DSC analyzer. Temperatures of the resin systems during the curing process were also monitored at varying amount of resins. Additionally, bending and tensile strength of the epoxy resins was measured to examine the mechanical stabilities for stone conservation. It was thus suggested that several compositions of epoxy resins were developed to control the curing kinetics and consequently temperature of the system.

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발표코드: II-POLY.P-72

발표분야: 고분자화학

발표종류: 포스터, 발표일시: 목 15:00~17:00

Hyaluronic acid-Catechol Conjugates: pH-dependent Mimicking of Mussel Adhesive Proteins by Adhesive Surface Coating vs. Cohesive Hydrogels

홍선기, 이해신

KAIST 화학과

Hyaluronic acid (HA) is a biocompatible polysaccharide that has been widely used as biomaterials. Until now, many hyaluronic acid hydrogel have been developed by chemical reactions, but there is no research using hyaluronic acid derivatives for direct interaction with variety of substrate. Herein, we demonstrated a new approach to design hyaluronic acid derivative (HA-catechol) with dual properties, adhesive to surface and cohesive to each polymer, by mimicking the unique functional group of mussel-adhesive proteins. In acidic pH condition, the synthesized polymers were adherent on a variety of substrates including ceramics, metal & metal oxide, and synthetic polymers, resulting the superhydrophilic surface modification, Whereas in basic pH condition, they were cohesive to each other forming hydrogel. Our new designed hyaluronic acid derivative plays a role as a bridge between the surface science and bulk materials science, two major research areas of biopolymers. We expect our investigation contribute on the development of a brand-new soft matter on the interface between surface and bulk system.

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발표분야: 고분자화학

발표종류: 포스터, 발표일시: 목 15:00~17:00

Optical and photorefractive Properties of hole-conductor polymer based composite for Holographic Applications.

지석환, 최철성, 김낙중

한양대 화학과

The photorefractive (PR) effect is a spatial modulation of the refractive index of a material upon illumination of a non-uniform beam through photoconductivity and electro-optic (EO) properties. When two coherent beams intersect a PR material, the internal space-charge field is formed due to the redistribution of the photogenerated charge generate that subsequently modulate the refractive index via an EO effect. The photorefractive composite is composed with several components such as photoconducting polymer, sensitizer, non-linear optic (NLO) chromophore and plasticizer. Photoconducting polymer and sensitizer related to charge generation, transport and trapping processes. NLO chromophore is an important factor to perform a good photorefractivity because orientational of NLO chromophore determines EO properties of the PR composite. Plasticizers are used in order to lower the glass transition temperature (T_g) of the composites down to the room temperature. We investigate the photorefractive properties such as photocurrent, diffraction efficiency and PR response time using several photorefractive composites.

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장소: 제주ICC

발표코드: II-POLY.P-74

발표분야: 고분자화학

발표종류: 포스터, 발표일시: 목 15:00~17:00

Electro-optical properties of electrochromic devices from the conducting polymer nanopattern

김유나, 김은경

연세대 화학공학과

Poly(3-hexylthiophene) (P3HT) films were patterned by a soft lithography technique using a nanopatterned PDMS mold to generate submicron size gratings. It was found that the diffusion coefficient of ions in the patterned electrode was much larger than that of the pristine P3HT electrode. As a result of such facilitated counter anion diffusion associated with redox processes at the P3HT electrode, electrochromic (EC) properties of the nanopatterned P3HT electrode were greatly enhanced. Using 1D patterned cell, light polarization properties were studied in colored and bleached states. Depending on the pattern direction, polarized diffraction was achieved via an electrochromic operation. The highest diffraction efficiency and dichroic ratio were obtained from 0 degree at colored state.

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발표코드: II-POLY.P-75

발표분야: 고분자화학

발표종류: 포스터, 발표일시: 목 15:00~17:00

Enhanced Buffering Capacity and Gene Transfection Efficiency by Conjugating Imidazole Containing Amino Acids to Poly(amidoamine) Dendrimers

유광식, 배윤미, 최혜, *최인성, 최준식

충남대 생화학과 *KAIST 화학과

Cationic polymers such as PEI, PAMAM and PLL have been widely investigated and developed for deliver the genetic materials to nucleus. Conventional vector systems have several obstacles to overcome such as low transfection efficiency and cytotoxicity. To achieve better gene transfection efficiency and less cytotoxicity, PAMAM dendrimers have been subjected to numerous chemical modifications to obtain more effective and less toxic to cells. In this study, we introduced histidine residues successively to L-arginine grafted PAMAM G4 dendrimers (PAMAM G4-Arg) which has been synthesized and investigated in our previous study. Introducing histidine residues to conventional polymer vector systems could be effective to enhance their durability against acidic environment such as lysosome. Synthesized PAMAM G4 derivatives (PAMAM G4-His(1, 2, 3)-Arg) effectively delivered pDNA into the cells and transfection efficacy improved impressively as the number of histidine elongation increased. Acid-base titration results showed that improvement of buffering ability in a pH range of 3.5 to 6 as the number of histidine residues increased. Gene transfection and cytotoxicity of the PAMAM G4 derivatives were examined using various cell lines and they showed improved properties compared to native PAMAM G4 and PAMAM G4-Arg dendrimers. Also, confocal microscopy study showed that His(1, 2, 3)-Arg peptide containing PAMAM G4 dendrimer derivatives effectively delivered pDNA into cell. Overall, we suggest that introducing histidine residues to PAMAM G4-Arg dendrimer could be a promising strategy for the delivery of genetic materials via non-viral vector system.

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발표코드: II-POLY.P-76

발표분야: 고분자화학

발표종류: 포스터, 발표일시: 목 15:00~17:00

Bulk heterojunction solar cells using low-band gap semiconducting polymers containing arylene unit as a crystallization inducing group

김지훈, *진성호, **신원석, ***윤성철, 황도훈

부산대 화학과 *부산대 화학교육과 **한국화학연구원 에너지소재연구센터 ***한국화학연구원
화학소재연구단

A series of electroactive and photoactive conjugated copolymers based on Fluorene and Benzothiadiazole, arylene units polymers were synthesized using a Suzuki coupling polymerization by controlling the monomer ratios. The ratio of arylene units in copolymers decreased the peak and onset absorption of the copolymers moved to longer wavelength region so that band gap energies became smaller. . The resulting copolymers were characterized by ¹H- and ¹³C-NMR, elemental analysis, DSC, and TGA. These copolymers were found to be soluble in common organic solvents and are easily spin-coated onto glass substrates, resulting high optical quality thin films without defects. Thermo gravimetric analysis shown the copolymers have high thermal stability, the 5 % degradation temperature was found about 350 °C. The LUMO energy levels of the copolymers are well matched PCBM LUMO energy level, which ensures the efficient electron flow. The bulk heterojunction solar cell were made by the following configuration ITO/PEDOT:PSS/PFDTBT-10 arylene: PC71BM/TiO_x/Al, the active layer was sandwiched between hole injecting PEDOT:PSS layer and hole blocking TiO_x layer, the maximum power conversion efficiency (PCE) was 3.16 % with short circuit current density (J_{sc}) of 9.61 mA/cm², open circuit voltage (V_{oc}) of 0.81 V and fill factor (FF) of 32 %.

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발표코드: II-POLY.P-77

발표분야: 고분자화학

발표종류: 포스터, 발표일시: 목 15:00~17:00

Cell Adhesion Behavior on Charged Gradient Surfaces with Variation of Compositions of Carboxyl and Amine End-Groups

KHATUA DIBYENDU

서강대 화학과

Understanding the cell behavior on biomaterial surfaces is important in tissue engineering and biomedical industry because biomaterial plays a key role in cell behavior. For example, a stem cell can be differentiating into specialized cell types, through cell division under different culture conditions, provided by a specific surface. However, designing of the specific bio-surfaces on which target cells can be cultured, is very difficult. Gradient surfaces can be a very efficient platform to evaluate the favorable surface condition for the cellular function because the effect of one or more selected surface properties can be tuned in a single surface under identical experimental conditions. Among the surface properties, biophysical properties coming from surface charge variations have been gained a considerable attention, because these parameters have been found to affect critically the cellular behavior. In this presentation, we prepared two-component mixed self-assembled monolayer gradient (methyl-carboxyl, methyl-amine) surfaces. Water contact angle, atomic force microscopy, X-ray, and X-ray photoelectron spectroscopy techniques have been used to characterize the prepared surfaces. We studied the adhesion, and proliferation of different types of cells on these surfaces.

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발표코드: II-POLY.P-78

발표분야: 고분자화학

발표종류: 포스터, 발표일시: 목 15:00~17:00

Adsorption behavior and fibro genesis of Fibronectin on negatively charged-patterned surfaces

Yalda Hozhbari Pooladi Nezhad, *신관우

서강대 화학과 *서강대 화학과 및 바이오융합과정

Fibronectin(FN) is a high molecular extracellular glycoprotein that is found as globular or extended fibril structures depending on biological conditions. When it converts to the fibril structure at the cellular membrane surface, FNs play a critical role in angiogenesis, differentiation, proliferation, migration, wound healing and tissue repairing. Previously, we found that FN can selectively adsorb onto a highly charged surface, and FNs form a micro-scaled stretched fiber network. In this study, we are trying to find essential parameters, providing i) how the water-soluble FNs can self-assembled to be the insoluble fibers, ii) how individual fibers can physically recognize neighboring fibers to form a fiber network, and iii) finally, how shapes, and patterned sizes of the charged surface can influence the physical properties of adsorbed FN fibers (size, and direction of fiber formation).

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장소: 제주ICC

발표코드: II-POLY.P-79

발표분야: 고분자화학

발표종류: 포스터, 발표일시: 목 15:00~17:00

New Asymmetric Blue Emitters Based on Phenylanthracene Core for OLEDs : Syntheses, Processability, and Electroluminescent Properties

이대희, 김현경, *박종욱, **정민철, 이지훈

충주대 나노고분자공학과 *가톨릭대 화학과 **순천대 화학공학과

최근 각광을 받고 있는 Organic Light Emitting Diodes(OLED)는 재료 측면에서 크게 저분자와 고분자로 분류된다. 저분자는 정제가 용이하며 효율과 수명면에서 고분자에 비해 뛰어나지만, 소자를 제작함에 있어 증착이라는 방법을 사용하기 때문에 대면적화에 어려움이 있다. 반면에 고분자는 Spin coating 방법을 사용하여 대면적화에 유리하지만, 증착을 하는 저분자에 비해 효율과 수명이 낮으며, 정제에 큰 어려움이 있다. 따라서 여기에선 저분자와 고분자의 장점인 정제가 용이하며, 증착과 Spin coating을 이용한 소자 제작이 모두 가능한 페닐나프탈렌 코어를 가지는 새로운 저분자 비대칭 청색 OLED 발광재료의 합성과, Side group의 치환기 위치에 따른 광학적, 열적, 전기화학적, 전계발광적 특성의 변화를 체계적으로 조사하였다.

일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: II-POLY.P-80

발표분야: 고분자화학

발표종류: 포스터, 발표일시: 목 15:00~17:00

Novel D-A- π -A Coumarin Dyes Containing Low-Band-Gap Chromophores for Dye-Sensitized Solar Cells

서강득, 최인택, 김환규

고려대 신소재화학과, 태양광정보소재 연구센터

A series of coumarin dyes containing a low-band-gap chromophore of benzothiadiazole, which comprises a coumarin moiety as the electron donor and a cyanoacrylic acid moiety as electron acceptor in D-A- π -A system, were developed to use in dye-sensitized solar cells (DSSCs). The introduction of benzothiadiazole unit into the molecular frame distinctly makes the narrow bandgap between the highest occupied molecular orbital (HOMO) and the lowest unoccupied molecular orbital (LUMO), thus red-shifting the absorption peak. Their chemical structures were characterized by ^1H -NMR, FT-IR, UV-vis absorption, and FAB-mass spectroscopies. Their electrochemical properties were studied by cyclic voltammetric measurement. The ground state geometries of the dyes have been optimized by DFT. The synthesis and characterization of organic D-A- π -A system coumarin dyes containing electron-withdrawing benzothiadiazole for dye-sensitized solar cells will be presented.

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장소: 제주ICC

발표코드: II-POLY.P-81

발표분야: 고분자화학

발표종류: 포스터, 발표일시: 목 15:00~17:00

Synthesis and Optical Property of Poly(trifluoroethylene-co-hexafluoropropylene)

이상구, *하종욱, **장봉준

충북대 화학공학과 *한국화학연구원 계면화학공정팀 **한국화학연구원 환경자원연구센터

Fluorinated polymers exhibit a number of interesting properties such as low refractive index, high transmittance, and low surface free energy. In this study, we report on optical property of poly(trifluoroethylene-co-hexafluoropropylene)(P(TrFE-co-HFP))films. To observe transmittance and refractive index of copolymer film, spin-coated films on glass slide were crystallized by cooling from 200 °C. It was found that the HFP content in the polymer chains influenced refractive index of their thin films. As increasing the HFP content in polymer chains, refractive index was decreased.

일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: II-POLY.P-82

발표분야: 고분자화학

발표종류: 포스터, 발표일시: 목 15:00~17:00

Synthesis of gene carriers using cationic polymer based on polydiacetylene liposomes and their applications

임강혁, 최혜, 최준식

충남대 생화학과

In this study, polyethylenimine was used for gene carrier because of its cationic property and DNA condensability. Also polyethylenimine with high molecular weight shows high gene delivery efficiency, but its toxicity is high, too. Polydiacetylene liposomes are made of diacetylene lipid monomers. These liposomes can be polymerized by ultraviolet irradiation. Also we can observe the color transition of polydiacetylene liposomes by various environmental stimuli. These characteristics have been utilized as chemical or biological sensor systems. It's too difficult to complex with DNA because of its anionic surface. So, to remedy polydiacetylene liposome's shortcomings, these liposomes will be conjugated with polyethylenimines as a liposomal vector for gene delivery. We confirmed the complexation polymeric liposome with DNA and then performed transfection and cytotoxicity assay. As the result, these cationic liposomal carriers showed significant gene transfection efficiency and low cytotoxicity. This study shows that polyethylenimine-conjugated polydiacetylene liposomes are expected to be an efficient gene carrier system.

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장소: 제주ICC

발표코드: II-POLY.P-83

발표분야: 고분자화학

발표종류: 포스터, 발표일시: 목 15:00~17:00

Investigating polaron dynamics in newly synthesized carbazole-C60 derivative blended polymer photovoltaic device

이창렬, *강남구, **Neil Greenham, ***이재석, 황인욱, ****한송희

광주과학기술원 고등광기술연구소 *Department of Chemistry, University of Massachusetts Lowell

Cavendish Laboratory, University of Cambridge *광주과학기술원 신소재공학과 ****목포해양대

교양과정부

The optical properties and polaron dynamics of newly synthesized polycarbazole-C60 derivative (C5C60) blended polymer photovoltaic device were investigated by quasi steady-state photo-induced absorption (PIA) spectroscopy. The polycarbazole was covalently connected with C60 and the content of C60 was 5.4 mol% in C5C60. From time-correlated single photon counting and room temperature PIA experiments, PL quenching of carbazole moiety in C5C60 was associated with the exciton dissociation between polycarbazole and C60. A broad PIA spectrum centered at 750nm (1.36V), which is assigned as the polaron state of carbazole of C5C60 was observed at room temperature PIA experiments. The C5C60 showed the good electron accepting properties when blended with conjugated polymer (MEH-PPV). The exciton lifetime of MEH-PPV was changed from ~200ps to 40ps by blending C5C60. The polaron peak at 825nm, which is assigned as the polaron state originated from the MEH-PPV and C5C60, was observed at room temperature PIA experiments. From the spectroscopic results, the C5C60 could be used as good electron acceptor when blended with conjugated polymer. The characteristics of mobility and the photovoltaic device performance are under investigation.

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장소: 제주ICC

발표코드: II-POLY.P-84

발표분야: 고분자화학

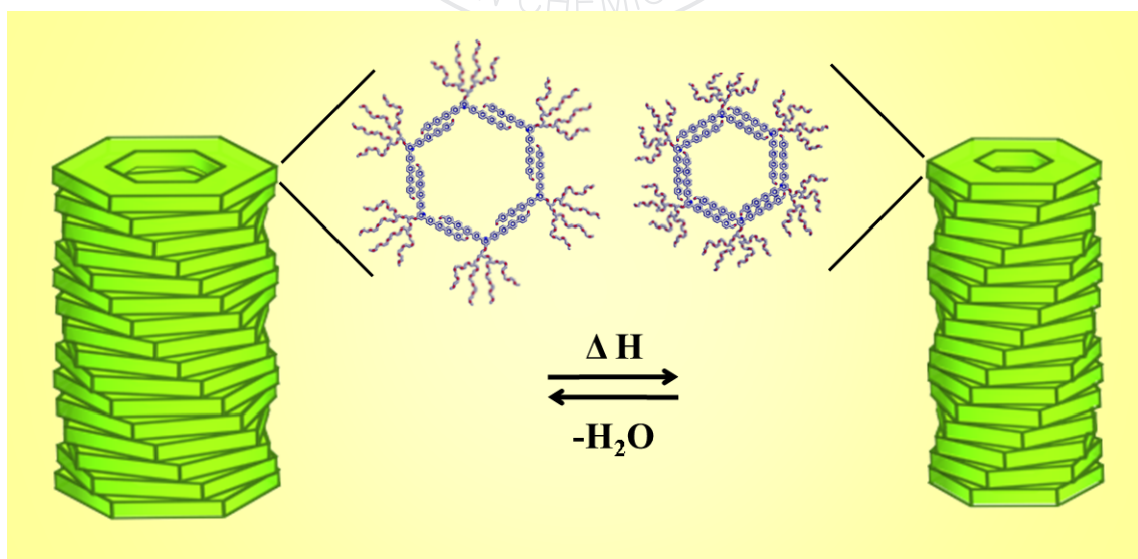
발표종류: 포스터, 발표일시: 목 15:00~17:00

Reversible Rotation like Breathing Motion in Tubular Assembly of Hexameric Macrocycles

황철강, *김태훈, 이명수

서울대 화학과 *서울대 화학부

We have synthesized bent-shaped aromatic amphiphile containing meta-linked pyridine segment and oligoether dendrons. It self-assembles into an elongated tubular structure with an internal diameter of 3~4 nm through π - π stacking and electrostatic interactions. The most notable feature of the tubular aggregates investigated is thermodynamic motion like breathing with reversible rotation of tubular stacking. This structural transition is accompanied by reversible hydrogen bonding between pyridine and water. Such cylindrical aggregates with dynamic structural changes may provide a new strategy for creating intelligent nanomaterials with internal channels.



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발표코드: II-POLY.P-85

발표분야: 고분자화학

발표종류: 포스터, 발표일시: 목 15:00~17:00

Novel Zn(II)-porphyrin Derivatives with D- π -A Structures for Highly Efficient Dye-Sensitized Solar Cells

이명준, 강민수, *김환규

고려대 소재화학과 *고려대 신소재화학과

We have designed and synthesized novel zinc porphyrin dyes that have D- π -A system containing a triphenylamine electron-donating group and a meso-substituted phenyl carboxyl anchoring group attached at the meso position of the porphyrin ring, yielding the push-pull porphyrins as the most efficient green dye for DSSCs applications. The synthesis and characterization of novel D- π -A system based on zinc-porphyrin derivatives will be investigated through the study of their photophysical and photoelectrochemical properties.

일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: II-POLY.P-86

발표분야: 고분자화학

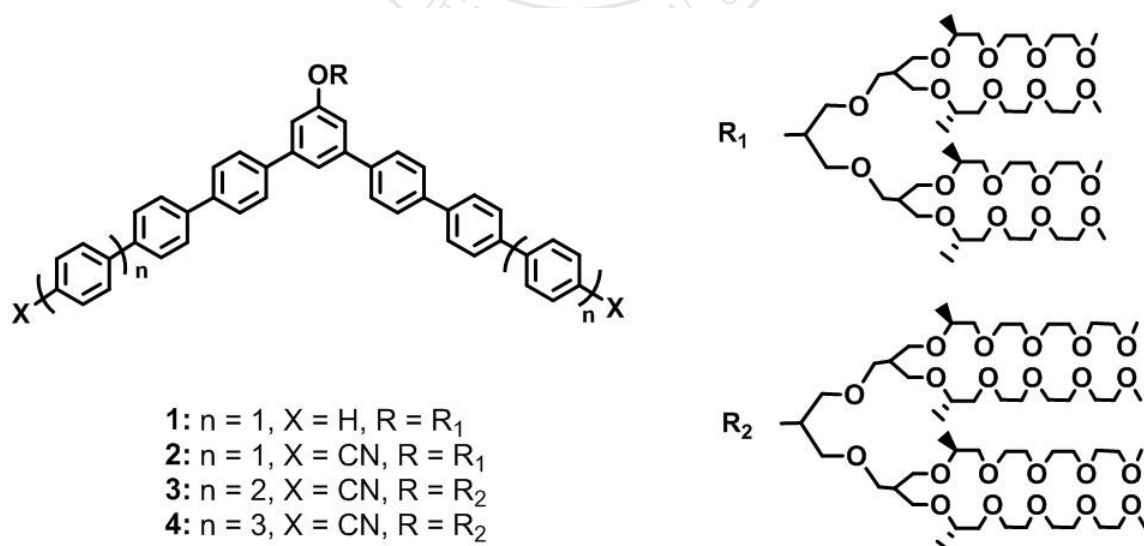
발표종류: 포스터, 발표일시: 목 15:00~17:00

Self-Organized Channel Structures from Non-covalent Macrocycles

강성균, *이명수

서울대 화학부 *서울대 화학과

Among the various supramolecular nanostructures, construction of channel-like structure has been received an enormous attention due to their application potential to electro-optic materials, biological channels, and nano-patterning processes. Especially, rod-coil block molecules consisting of rigid aromatic rod and flexible coil segments are excellent candidates for creating well-defined supramolecular structures via a process of spontaneous organization. We present here the formation of columnar structure with an amorphous channel from hierarchical assembly of diblock molecules consisting of a bent-shaped aromatic segment and an aliphatic dendritic segment.



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장소: 제주ICC

발표코드: II-POLY.P-87

발표분야: 고분자화학

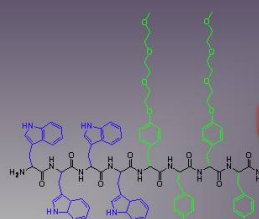
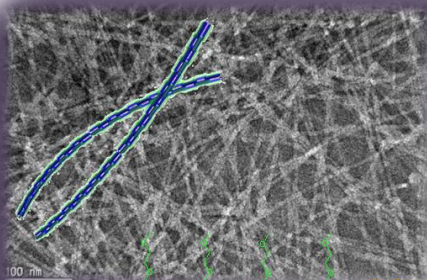
발표종류: 포스터, 발표일시: 목 15:00~17:00

Understanding of Nanostructure from Amphipathic Peptides by Different Molecular Designs

박일수, 이명수

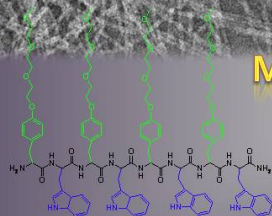
서울대 화학과

We have synthesized two kinds of amphipathic peptides which are different about sequence. One type is alternative sequence 'ABABAB', another type is diblock sequence 'AAABBB'. DLS study and TEM study show that they form nanostructures in water. The peptides having alternative sequence design form fiber-like structures. On the other hand, diblock peptides aggregate vesicles. To understand conformation of these, they were measured by CD study, IR study and TFE addition. These studies revealed that the conformation of alternative peptides is beta-sheet conformation. But, diblock peptides are similar to alpha-helix conformation. These differences can be explained that differences of molecular design make contrast of phase separation between alternative sequence and diblock sequence. We can expect that various nanostructures can be made by simple differences of molecular designs.

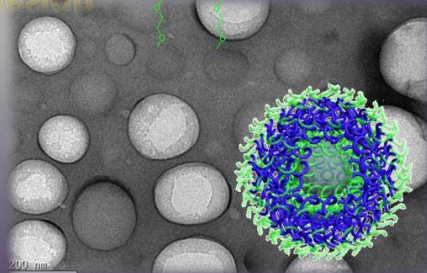


Diblock Peptide

Molecular Design



Alternative Peptide



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장소: 제주ICC

발표코드: II-POLY.P-88

발표분야: 고분자화학

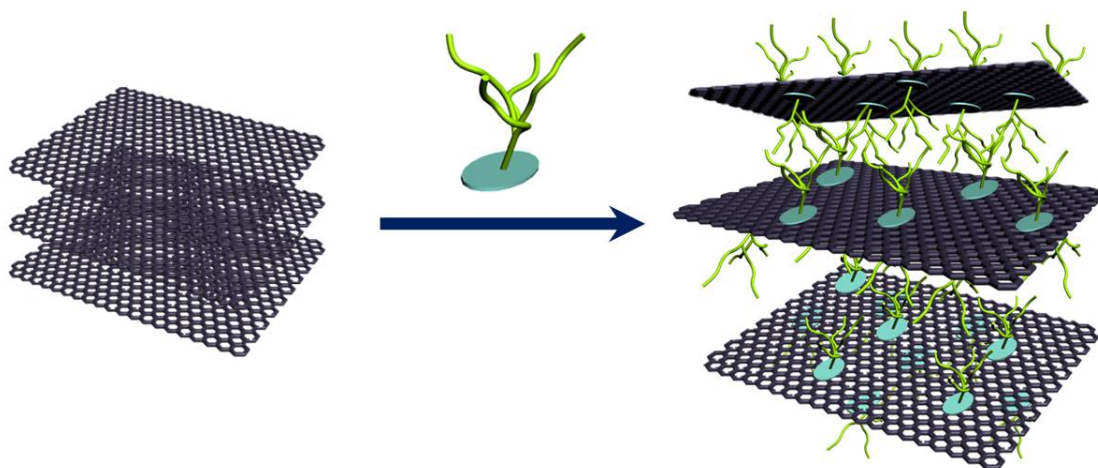
발표종류: 포스터, 발표일시: 목 15:00~17:00

Amphiphilic Pyrene Sheet for Selective Functionalization of Graphene

이동우

서울대 화학부

We have demonstrated that aromatic amphiphile consisting of a hydrophilic dendron and an aromatic segment with a planar conformation can selectively exfoliate graphite powder into single- and double-layer graphene sheets in aqueous solution through hydrophilic functionalization of graphene surfaces. The graphene dispersions showed to be highly stable over 2 months without any noticeable sedimentation and aggregation. Spin coating and then drying of the dispersions give rise to a transparent film that shows good electrical properties.



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발표코드: II-POLY.P-89

발표분야: 고분자화학

발표종류: 포스터, 발표일시: 목 15:00~17:00

Synthesis of Well-Defined (Nitrilotriacetic Acid)-End-Functionalized Polystyrenes and Their Bioconjugation with Histidine-tagged Green Fluorescent Proteins

Mohammad Abdul Kadir, 김봉수, 백현종

부산대 고분자공학과

We have synthesized nitrilotriacetic acid end-functionalized polystyrene (NTA-PS) for the controlled bioconjugation with histidine-tagged green fluorescence proteins (His6-GFP). NTA-PS was prepared using initiators containing t-butyl protected NTA moiety via atom transfer radical polymerization (ATRP) of styrene; the protected t-butyl group was subsequently removed at the α -chain end of polystyrene. The structure of NTA-PS was characterized using ^1H NMR, ^{13}C NMR, and GPC. NTA chain ends of the polystyrenes were complexed with Ni^{2+} to produce Ni-NTA-PS, which produced well defined micelles of 60-80 nm with His6-GFP in water/DMF and the size of micelles decreased to 45-60 nm when excesses imidazole was added.

일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: II-POLY.P-90

발표분야: 고분자화학

발표종류: 포스터, 발표일시: 목 15:00~17:00

Stimuli-Responsive Copolymers by Atom Transfer Radical Polymerization of Methacrylates

김병재, 김봉수, 정종화, *김진구, **정기석, 백현종

부산대 고분자공학과 *이리도스주식회사 **이리도스주식회사 R&D 팀

pH- and temperature-responsive semiblock-polymers, poly[2-(2-methoxyethoxy) ethyl methacrylate]-*block*-poly[2-(dimethylamino)ethyl methacrylate] (PMEO2MA-*b*-PDMAEMA), have been synthesized via Atom transfer radical polymerization (ATRP). Amine groups of DMAEMA are selectively quaternized with benzyl chloride(QDMAEMA). Ethyl 2-bromoisobutyrate (EBiB) was used as initiator and CuCl/2,2-bipyridine,bpy, as a complexing ligand. The copolymers were characterized by proton nuclear magnetic resonance (^1H NMR), gel permeation chromatography (GPC). Behavior of stimuli-responsive copolymers was studied in aqueous solution by measuring the lower critical solution temperature (LCST) using UV/vis spectroscopy. In this study, the measurements performed at pH 4, pH 7 and pH 10. These copolymers exhibit a reproducible temperature-responsive behavior. LCST is tunable by the number of quaternization and pH.

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장소: 제주ICC

발표코드: II-POLY.P-91

발표분야: 고분자화학

발표종류: 포스터, 발표일시: 목 15:00~17:00

Syntheses and Characterization of Vacuum-Depositable and Solution-processable New HOST Materials based on Dialkoxylated Biphenyl Derivatives for PHOLEDs

이남진, 이대희, 김현경, 인인식, 이지훈

충주대 나노고분자공학과

유기 전계 발광 소자(Organic Light-Emitting Diodes)는 형광성 또는 인광성 유기 화합물 박막에 전류를 흘려주면, 전자와 정공이 유기막에서 결합하면서 빛이 발생하는 현상을 이용한 능동 발광형 표시 소자로서, 경량, 부피가 간소하고 제작공정이 간단하고 고화질에 넓은 시야각이 특징으로 최근들어 급속도로 발전하고 있는 분야이다. 발광층 형성 재료는 발광 메커니즘에 따라 일중항 상태의 엑시톤을 이용하는 형광 재료와, 삼중항 상태의 엑시톤을 이용하는 인광 재료로 나뉜다. 형광 재료를 이용하는 유기 EL 소자는 생성되는 엑시톤의 에너지 중 75%는 전혀 이용되지 않는다. 그렇기 때문에 인광 재료를 사용하여 발광효율을 높이려는 연구가 진행되고 있다. 본 연구는 새로운 HOST 재료설계에 가장 기본적으로 사용하는 Carbazole의 특성변화를 개선하는데 기초를 두었다. Carbazole의 경우 3,6-위치가 electrochemically active 하여 산화가 되거나 또는 Hole이 많이 생성되어 주위가 electron deficient 분위기에 놓이게 될 때 쉽게 dimer를 형성할 수 있다. 결과적으로 HOST 분자의 에너지준위의 변화가 초래되고 특히 Blue 인광시스템에서의 Dopant로의 Energy Transfer가 비효율적으로 진행되어 결국 소자의 degradation과 수명 단축을 초래한다. 이러한 Dimer 형성을 제거하기 위해 Carbazole 3,6-번 위치에 Blocking side group을 도입함으로써 열적 안정성과 박막안정성 및 전기적 안정성이 개선된 새로운 HOST 재료를 합성하였고 이들 재료의 Electrophosphorescent OLEDs (PHOLEDs) 소자를 제작하여 그 특성에 대해 조사하였다.

일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: II-POLY.P-92

발표분야: 고분자화학

발표종류: 포스터, 발표일시: 목 15:00~17:00

Crack Healing in a Polymeric Material by microwave irradiation

임예지, *유미란, 정찬문

연세대 화학과 *Yonsei University

The object of this study is to develop an intelligent polymeric material in which cracks can be readily healed by microwave irradiation. The reaction by microwave irradiation has advantages such as better process control, faster curing times, and higher yields compared with the reaction by conventional heating. Perfluorocyclobutane (PFCB)-containing polymers have been studied as a unique class of fluoropolymers having excellent properties such as low dielectric constant, good thermal stability, high Tg, and optical transparency. In this work, the potential of a PFCB polymer as a mendable material was investigated by means of microwave irradiation. Crack were generated in PFCB polymer specimens, and a part of the cracked samples were healed by microwave re-irradiation. The crack-healing ability of the polymers was investigated by FT-IR. The crack healing in the polymers was successfully demonstrated by the measurement of flexural strength of the polymer specimens before and after healing.

일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: II-POLY.P-93

발표분야: 고분자화학

발표종류: 포스터, 발표일시: 목 15:00~17:00

Europium(III)-cored Complexes as Wavelength Conversion Materials for Large Performance Enhancement on Dye-Sensitized Solar Cells

오정환, *송해민, *김상균, **주명종, *김환규

고려대 소재화학과, 태양광정보소재 연구센터(ITRC) *고려대 신소재화학과, 태양광정보소재 연구센터(ITRC) **고려대 신소재화학과

Eu(III)-cored complex was first investigated as a promising wavelength conversion coadsorbent to improve UV light harvesting through energy transfer from Eu^{3+} ions to TiO_2 films via dyes, which absorbs light at shorter wavelengths and emits light at longer wavelengths, for highly efficient dye-sensitized solar cells. Black dye/WCM-sensitized solar cell exhibits a superior device performance with the enhanced conversion efficiency by 1.22 times, under AM 1.5 sunlight.

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장소: 제주ICC

발표코드: II-POLY.P-94

발표분야: 고분자화학

발표종류: 포스터, 발표일시: 목 15:00~17:00

Photoreactive coatings for self-healing of microcracks

송영규, 조예현, 임예지, 유환철, 정찬문

연세대 화학과

Polymeric materials are used in a variety of applications, but they are susceptible to damage induced by various physical and chemical factors. This results in microcrack formation and propagation, ultimately leading to significant reduction in mechanical performance and other desired properties of the materials. Recently, much attention has been paid to crack healing in polymeric matrixes. In this work cinnamate-containing siloxanes were synthesized as healing agents and their applicability to crack healing was investigated. Siloxane methacrylates were also investigated as healing agents.

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장소: 제주ICC

발표코드: II-POLY.P-95

발표분야: 고분자화학

발표종류: 포스터, 발표일시: 목 15:00~17:00

Synthesis and Characterization of New Isomeric Polymers based on Benzo[c][1,2,5]thiadiazole Derivatives for PLEDs : Its Optical, Thermal, and Electroluminescent Properties

정훈섭, 인인식, *박종욱, 이지훈

충주대 나노고분자공학과 *가톨릭대 화학과

PLEDs (Polymer Light-Emitting Diodes)는 저분자 OLEDs 에 비해 분자량이 큰 Homopolymer 또는 Copolymer 형태로 spin-coating, inkjet printing 등의 용액공정으로 제작함에 따라 Large-area flat panel displays, Flexible display 등 차세대 Display 활용에 보다 용이하다. 또한 저분자 OLEDs 에 비해 우수한 열안정성을 가지고 있다. 그러나 지금까지 저자가 알기로는 고분자 주쇄에 존재하는 isomeric segment 에 의해 고분자의 물성의 차이가 있다는 것에 대한 연구보고는 거의 없었다. 이에 Isomeric polymers 에 따른 물성의 차이점을 조사하기 위하여 Benzo[c][1,2,5]thiadiazole 를 분자 Core 구조로 두고 Side-groups 의 위치가 각각 up-up / up-down 의 isomeric monomer 을 합성하였다. 각각의 Isomeric polymers 는 Suzuki 또는 Yamamoto aryl-aryl coupling 을 이용하여 Homopolymers 또는, 적절한 Comonomer 를 이용하여 Copolymers 합성하였다. 얻어진 polymers 은 UV-Vis., NMR, GPC 등을 통하여 구조분석을 하였으며, 구조간 차이를 조사하기 위해 광학적, 열적, 및 유기발광소자의 전기적인 특성을 비교 분석하였다.

일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: II-POLY.P-96

발표분야: 고분자화학

발표종류: 포스터, 발표일시: 목 15:00~17:00

Preparation of urea-formaldehyde microcapsules containing siloxane methacrylate as a photoreactive healing agent

조예현, 임예지, 송영규, 정찬문

연세대 화학과

The preparation of microcapsules for application in the fabrication of self-healing composites has been paid more attention. The microcapsules must possess sufficient strength to remain intact during processing of the host polymer, yet rupture when the polymer is damaged. High bond strength to the host polymer combined with a moderate strength microcapsule shell are required. To provide long shelf-life the capsules must be impervious to leakage and diffusion of the encapsulated healing agent for considerable time. A series of microcapsules were prepared by in situ polymerization method with poly(urea-formaldehyde) as a shell material and a siloxane methacrylate-containing compound as a core material. The methacrylate-containing compound can be used as a photoreactive healing agent. The chemical structure of microcapsule was characterized using infrared spectroscopy. The size, size distribution, morphology, and wall thickness were controlled by processing parameters such as agitation rate and core-shell ratio, and they were characterized by optical microscopy and scanning electron microscopy (SEM). Thermal properties of capsule, shell and core were investigated by TGA.

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장소: 제주ICC

발표코드: II-POLY.P-97

발표분야: 고분자화학

발표종류: 포스터, 발표일시: 목 15:00~17:00

Preparation of Well-defined Polymeric Dispersants for Pigment by Atom Transfer Radical Polymerization

정종화, 김병재, *김은희, **정기석, ***김진구, 백현중

부산대 고분자공학과 *(주)솔켄 기술연구소 **이리도스주식회사 R&D팀 ***이리도스주식회사

Recently, polymeric dispersants have been extensively used in various fields such as paints, inks, CNTs, displays, etc. The chemical structure of polymeric dispersants for pigment has an important role to improve dispersion stability and prevents aggregation or flocculation of pigment in organic or aqueous solvent system. Polymeric dispersants should contain both the anchoring group that interacts on pigment surface and with stabilizing group that provides entropic stabilization. In this study, we investigated the interaction between different polymeric dispersants and pigment blue. For the purpose, we synthesized well-defined various block copolymers containing prenominate two groups with different molecular weight and composition by atom transfer radical polymerization (ATRP). The synthesized block copolymers were characterized by gel permeation chromatography (GPC) and ^1H NMR spectroscopy.

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장소: 제주ICC

발표코드: II-POLY.P-98

발표분야: 고분자화학

발표종류: 포스터, 발표일시: 목 15:00~17:00

Preparation of Porous Thin Films of Aliphatic Polyimides

유환철, *S. Vijay Kumar, **Kazuaki Kudo, **Jiyoung Choi, 정찬문

연세대 화학과 *Department of Chemistry, Yonsei University **Institute of Industrial Science, University of Tokyo

Fully aliphatic polyimides (APIs) were prepared from rel-(1'R,3S,5'S)-spiro[furan-3(2H),6'-[3]oxabicyclo[3.2.1]octane]-2,2',4',5(4H)-tetrone (DAn) as dianhydride, and either cis-trans-1,4-diaminocyclohexane (mix-DACH) or trans-1,4-diaminocyclohexane (trans-DACH) as diamine. The solubility, optical transparency, and thermal properties of the polyimides were investigated. The solubility and decomposition temperature of the APIs were found to be correlated with their intermolecular regularity. Triblock copolyimides were synthesized through the incorporation of a thermally labile polymer, poly(propylene glycol) (PPG), into the APIs, and their thermal properties were studied. Nanoporous thin films of the full APIs were prepared via thermolysis of the labile block in the copolyimide films. Phase separation and nanopore formation in the copolymer films were confirmed via atomic-force microscopy (AFM) and scanning electron microscopy (SEM), respectively.

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장소: 제주ICC

발표코드: II-POLY.P-99

발표분야: 고분자화학

발표종류: 포스터, 발표일시: 목 15:00~17:00

Patterned fluorescence images in anthracene derivatives-containing films

이광훈, 송영규, 유환철, 정찬문

연세대 화학과

Patterned fluorescent images are applicable in displays, optical memory devices, sensors and imaging industries. The object of this study is to develop a technique of photoimaging using anthracene derivatives and their strong fluorescence. It is widely known that anthracene derivatives convert to corresponding dimers by UV irradiation above 300 nm. There are significant differences of fluorescent properties between their monomers and dimers. Consequently it was expected that their differences of fluorescence are applicable to fluorescence imaging. Fluorescence imaging using anthracene derivatives have advantages : only a small amount of them are needed for the imaging because they have strong fluorescent properties and versatile image patterns can be achieved depending on functional groups. The fluorescent properties of anthracene derivatives were investigated by UV and PL. The patterned images were successfully obtained and evaluated by fluorescence microscope.

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장소: 제주ICC

발표코드: II-POLY.P-100

발표분야: 고분자화학

발표종류: 포스터, 발표일시: 목 15:00~17:00

A study on voltage gain of the gravure printed SWNTs based TFTs as a function of the operating voltage

김다애

(주)파루 인쇄전자연구소

Many institutes have investigated printed thin film transistors (TFTs) to implement printed electronic logic circuits and devices. As printed electronic circuits become more complex, operating voltage and voltage gain of the printed TFTs are very important factors in the printed electronics. Because, the higher voltage gain and low operating voltage enable the integrated circuit design using less number of transistors. But due to intrinsic drawbacks of organic materials in terms of electronic properties, it is very difficult to reduce operating voltage and enhance voltage gain of the printed TFTs. In this research, we printed single walled carbon nanotubes (SWNTs) based TFTs using gravure printing processes to optimize electrical properties balance between operation voltages and voltage gain of the printed SWNTs based TFTs as a function of the operating voltage.

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장소: 제주ICC

발표코드: II-POLY.P-101

발표분야: 고분자화학

발표종류: 포스터, 발표일시: 목 15:00~17:00

Fluorescent Viscosity Sensor Application of Conjugated Polymer Film

이왕은, *이창렬, **곽기섭

경북대 고분자공학과 *광주과학기술원 고등광기술연구소 **경북대 공과대학/고분자공학과

The variation of fluorescence emission property of poly[1-phenyl-2-[p-(trimethylsilyl)phenyl]acetylene] (PTMSDPA) film according to the solvent viscosity at the swollen state was evaluated quantitatively. This polymer film quickly responded to various kinds of fluids, such as hydrocarbons, alcohols, and silicon oils, simply by putting them in contact with the films. The functional log-log equation of viscosity sensitivity of the PTMSDPA film was expressed as a linear equation of $\log(I/I_0) = C + x \log$. The probe-dependent constant (x) value of the present film sensor significantly varied according to the molecular affinity and size of the fluids. Especially, the x value for hydrocarbons was as high as 0.50. On the other hand, the x values for alcohols and silicon oils were relatively lower at 0.28 and 0.21, respectively.

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장소: 제주ICC

발표코드: II-POLY.P-102

발표분야: 고분자화학

발표종류: 포스터, 발표일시: 목 15:00~17:00

Novel Dual Functioned Coadsorbents for Highly Efficient Dye-sensitized Solar Cells

최인택, *김환규, *주명종, **송복주, ***강민수, *서강득, *김상균, *송해민

고려대 신소재화학, 태양광정보소재 연구센터(ITRC) *고려대 신소재화학과, 태양광정보소재 연구센터(ITRC) **고려대(세종) 신소재화학과, 태양광정보소재 연구센터(ITRC) ***고려대 소재화학과, 태양광정보소재 연구센터(ITRC)

Novel dual functioned coadsorbents (HC-Acids) have been systematically developed to use as an alternative to deoxycholic acid (DCA) in organic dye-sensitized solar cells (DSSCs). HC-Acids have a more bulky Y-shaped structure than DCA. Thus HC-Acids can act as a more effective spacer than DCA to remarkably suppress the π - π interaction of the dye molecules, which retards charge recombination, hence improving the performance of the DSSCs significantly. Furthermore, it also has the light harvesting effect at short-wavelength to improve electron injection yield into TiO₂ film, thus increasing J_{sc}. In other words, HC-Acids have dual function, such as the prevention of dye aggregation and the short UV light harvesting. As a result, power conversion efficiency of 8.89% , which is the highest efficiency obtained so far among DSSCs based on organic coumarin dye photosensitizers, was achieved under AM 1.5 G (J_{sc} = 17.25 mA cm⁻², Voc = 0.687 V, and FF = 74.93).

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장소: 제주ICC

발표코드: II-POLY.P-103

발표분야: 고분자화학

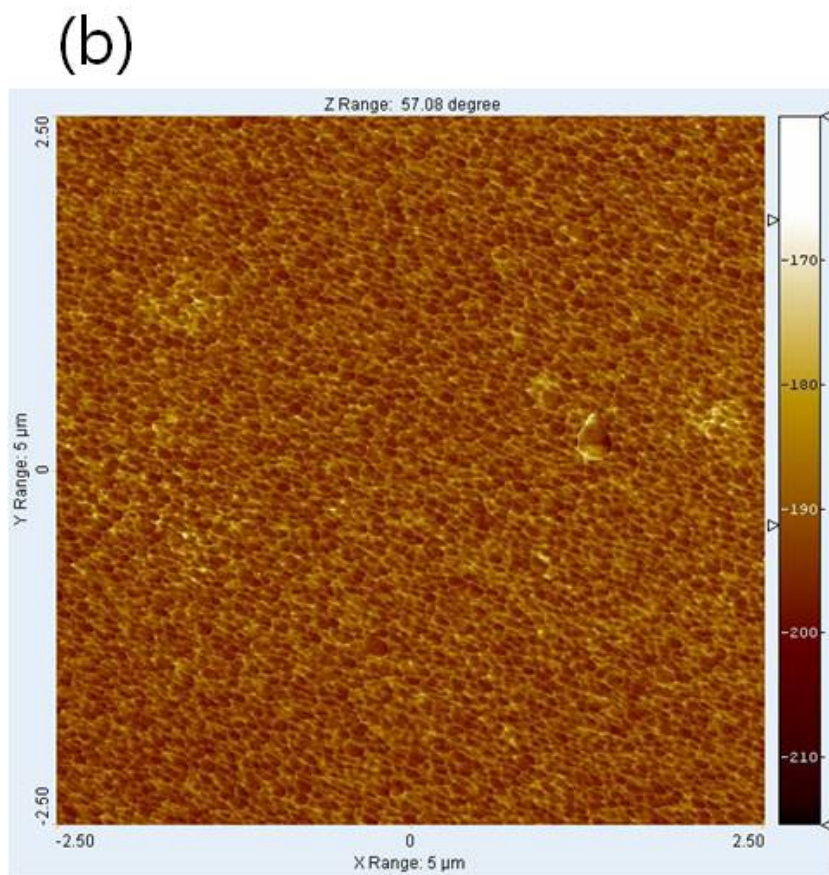
발표종류: 포스터, 발표일시: 목 15:00~17:00

Morphological characterization of multilayer in digital microfluidic chips

고효진, 권오선, *신관우

서강대 화학과 *서강대 화학과 및 바이오융합과정

We have fabricated and characterized the multilayer utilized for our digital microfluidic chips driven by electrowetting-on-dielectrics (EWOD). The multilayer of Teflon/parylene/ITO/SU-8 was prepared by using various coating techniques on a glass substrate in nano and micro thickness. The 2 μ m negative photoresist SU-8 with the designed pattern was deposited in the mask-aligner in UV photolithography. After that a 60 nm ITO electrode was sputtered via Ar plasma. For dielectrics, either parylene or Al₂O₃, was coated in 2 μ m thickness with the chemical vaporizing deposition method. For hydrophobic top coat a 200 nm Teflon AF 1600 was deposited by the spin coating method. Since SU-8 is the most important material in this multilayer, its 3D images of surfaces and structures have been extensively analyzed by AFM and SEM. We found that its surface roughness can be increased by O₂ plasma sputtering in a function of time and intensity. This plasma surface treatment clearly provides the aggregation of the SU-8. Then the surface will become more hydrophilic and remain for several months. Fig. 1 Multilayer in digital microfluidic chip driven by EWOD: (a) multilayer structure, (b) the AFM image of SU-8 2 before plasma treatment



일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: II-POLY.P-104

발표분야: 고분자화학

발표종류: 포스터, 발표일시: 목 15:00~17:00

Study on Gravure Printed Dielectric layer for All printed Thin Film Transistor

임소연

(주)지본

Gravure printing is considered a promised method for the manufacture of thin film transistors (TFTs) for the flexible and low cost electronics. To enhance performances and stability of the printed TFTs, gravure printer should provide fine patterns, surface morphology, and low surface roughness of the printed dielectric layer. In this study, dielectric layer was printed by R2P gravure printer on plastic films using dielectric inks (PD-100, Paru Company Korea) to achieve good patterns and low surface roughness for the gravure printed TFTs. And to invest the effects related to electrical performances of the printed TFTs, many factors of the gravure printing such as drying method, tension, printing velocity, ink conductivity and accuracy of pattern geometry are closely evaluated.

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장소: 제주ICC

발표코드: II-POLY.P-105

발표분야: 고분자화학

발표종류: 포스터, 발표일시: 목 15:00~17:00

Preparation, Properties, and Fluorescence Image Patterning of Acetylene-Acrylate Polymer Hybrid Film

박효상, 이대훈, *곽기섭

경북대 고분자공학과 *경북대 공과대학/고분자공학과

An acetylene-acrylate polymer hybrid film was successfully prepared by photopolymerization of UV-curable acrylic monomers in situ in the acetylene polymer film. This hybrid polymer film showed remarkable enhancement in emission, photooxidative stability as compared to the virgin acetylene polymer film. Also, a modified photolithography of this hybrid film using photomask in the process of photopolymerization produced a highly resolved, fluorescent image pattern on the film.

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장소: 제주ICC

발표코드: II-POLY.P-106

발표분야: 고분자화학

발표종류: 포스터, 발표일시: 목 15:00~17:00

Solid-State Polymerized Conducting Polymers for Highly Efficient, Iodine-Free Solid-State Dye-Sensitized Solar Cells

김정훈, *김병관, 김은경

연세대 화학공학과 *연세대 화공생명공학과

We developed a facile method for the preparation of iodine-free solid-state dye sensitized solar cells(ssDSSCs) with excellent performance and improved electrode/hole transporting material(HTM) interfacial properties based on the solid state polymerization(SSP) of a conductive polymer. The solid-state polymerizable monomer was small enough to effectively penetrate into the nanopores of TiO_2 film, improving interfacial contact between the electrode and HTM. Importantly, this approach allowed deep penetration of HTM into 11 μm thick TiO_2 film, allowing for enhanced dye adsorption and resulting in high performance. We believe that this SSP approach introduces a new and simple route toward the synthesis of conducting polymer as the HTM in iodine-free ssDSSCs serve as an alternative to the conventional photoelectrochemical polymerization method. Herein, we present about the application of highly conductive polymers to the I^2 free ssDSSCs with a facile fabrication method.

일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: II-POLY.P-107

발표분야: 고분자화학

발표종류: 포스터, 발표일시: 목 15:00~17:00

Study on fabrication of thin film transistors by applying Roll to Roll gravure process

한주경

(주)파루 인쇄전자연구소

Roll to Roll (R2R) gravure printing method is assured to be a simple way to fabricate flexible and ultra-low cost thin film transistors (TFTs). In this research, all R2R gravure printed TFTs were fabricated using silver nano-particle based conductive ink as an electrode, polymer binder-inorganic hybrid ink as a dielectric layer and SWNTs hybrid ink as an active layer. We evaluated several factors related to printing materials and processes such as fluidic properties of ink, thermal treatment, and web speed to accomplish high performance of printed TFTs. During discussion time, we will show the evaluation results such as effects of the printing layer thickness, roughness and uniformity of SWNTs network structure. As a result, all printed TFT shows 0.04cm²/Vs of mobility, 100 of on-off ratio in current, -6V of threshold voltage, and has p-type transistor properties. In addition, we printed a digital logic circuit which can generate 4 bits digital signal to show the possibility of all gravure printed Integrated Circuits (ICs) chip. This printed 4 bit digital logic circuit worked properly.

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장소: 제주ICC

발표코드: II-POLY.P-108

발표분야: 고분자화학

발표종류: 포스터, 발표일시: 목 15:00~17:00

Spectroscopic investigation of FRET molecular beacon for conjugated polymer-based DNA biosensors

정지은, *김보람, **우한영

부산대 나노소재공학과 *부산대 나노융합기술학과 **부산대 나노기술대학 나노정보소재공학과

Molecular beacons (MBs) are an oligonucleotide hybridization probe, which is a hairpin shaped molecule labeled with both of a 5'-fluorophore and 3'-quencher. Depending on the stem sequence of MBs, stability is changed and the resulting optical properties can be controlled. Additionally, the signal of fluorophore in the MBs can be amplified by using a conjugated polyelectrolyte via fluorescence resonance energy transfer (FRET). In this contribution, we investigated the photophysical properties of MBs having different stability in the presence of conjugated polymers with different hydrophilic and hydrophobic properties.

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장소: 제주ICC

발표코드: II-POLY.P-109

발표분야: 고분자화학

발표종류: 포스터, 발표일시: 목 15:00~17:00

Charge density effects on FRET to dye-labeled DNA in conjugated polymer based fluorescence

김보람, *정인환, *강미정, *심홍구, **우한영

부산대 나노융합기술학과 *KAIST 화학과 **부산대 나노기술대학 나노정보소재공학과

Poly(fluorene-co-phenylene) based CCPs with different charge density (per polymer repeat units) were synthesized and investigated as a fluorescence resonance energy transfer (FRET) donor to fluorescein-labeled single stranded DNA (ssDNA-FI). The newly synthesized CCPs show an identical electronic structure but obviously different water-solubility and the resulting optical properties such as molar absorption coefficient and PL quantum yield in aqueous solution. The FRET-induced FI signal was studied in detail in terms of charge density of the polymers, the resulting spectroscopic properties and the photo-induced charge transfer (PCT) quenching in the polymer/ssDNA-FI complex.

일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: II-POLY.P-110

발표분야: 고분자화학

발표종류: 포스터, 발표일시: 목 15:00~17:00

Novel Lanthanide(III)-chelated complexes based on Borondipyrromethane Ligands : Synthesis and Photoluminescence Properties

송복주, 김환규, *Jean-Claude G. Bünzli

고려대 신소재화학과 *École Polytechnique Fédérale de Lausanne

We have synthesized novel luminescent lanthanide complexes based on borondipyrromethane fluorophores(BODIPY-A; (Z)-methyl 4-((7-methoxy-4,5-dihydro-1H-benzo[g]indol-2-yl)(7-methoxy-4,5-dihydrobenzo[g]indol-2-ylidene)methyl)benzoic acid, BODIPY-B; (Z)-methyl 4-((7-methoxy-4,5-dihydro-1H-benzo[g]indol-2-yl)(7-methoxy-4,5-dihydrobenzo-[g]indolylidene)methyl)benzoic acid) derivatives for enhancing the emission intensity of lanthanide ion via efficient energy transfer from the excited state of the BODIPY based luminescent ligands to the lanthanide ions. The investigation results revealed that the lanthanide complexes have been optimized for the enhancement of emission intensity of lanthanide ion, namely the energy transfer process from the light harvesting chromophore to the emitting lanthanide ion, a high molar absorption coefficient, high fluorescence quantum yields, chemical and photochemical stability.

일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: II-POLY.P-111

발표분야: 고분자화학

발표종류: 포스터, 발표일시: 목 15:00~17:00

Multi Color Fluorescent Organic Nanoparticles for Bioimaging

서영훈, *김세훈, **장우동

연세대 화학과, KIST 의과학센터 *KIST 의과학센터 **연세대 화학과

In bioimaging, the development of highly fluorescent nanoparticles is of great importance. However, the substantial emission of common organic compounds becomes weak in the concentrated or aggregated states due to the intermolecular quenching interaction. Therefore, the preparation of compounds that emit efficiently in the solid state is recently under intense investigation. Herein, we have synthesized novel organic dyes exhibiting aggregation-enhanced fluorescence. The emission colors of organic dyes can be tuned in the range from blue to near-infrared modulating the chemical structure. We have demonstrated that organic nanoparticles with aggregation-enhanced fluorescence have great potential for bioimaging applications.

일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: II-POLY.P-112

발표분야: 고분자화학

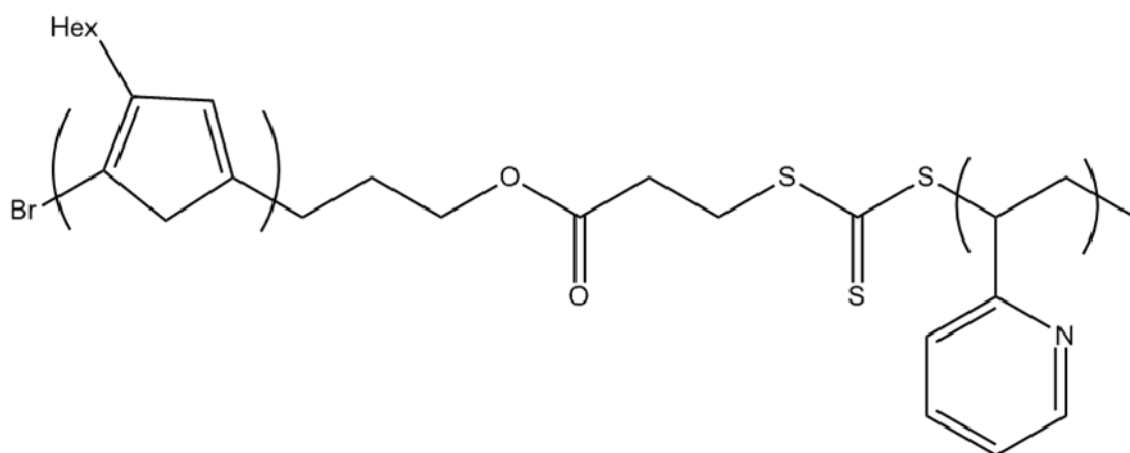
발표종류: 포스터, 발표일시: 목 15:00~17:00

Synthesis of Rod-Coil Block Copolymers for Organic Optoelectronics

정재연, *임현민, *명지은, 강영종

한양대 자연과학대학 화학과 *한양대 화학과

Block copolymers have been increasingly investigated due to their abundant morphology and versatile applications.[1]-[2] Especially rigid rod block containing copolymers have been of more interest recently because of their unique self-assembly behaviors which are quite different from conventional coil-coil type block copolymers. Alternatively, reversible addition fragmentation chain transfer polymerization (RAFT) is an attractive method for the synthesis of block copolymers because it does not involve the use of a transition metal catalyst.[3] In this presentation, we are going to report synthesis of rod-coil block copolymers containing poly 2-vinyl pyridine. This conductive block copolymer can assume different structures and a range of variational molecular weights and compositions, yielding new methods that can generate novel electronic and optical materials. Morphology changes and optical properties are characterized using SEM, TEM, PL and UV.[1] Lazzari, M., Liu, G., Lecommandoux, S., Eds. Block Copolymers in Nanoscience; Wiley-VCH: Weinheim, 2006.[2] O'Reilly, R. K.; Hawker, C. J.; Wooley, K. L. Chem. Soc. ReV. 2006, 35,1068–1083.[3] Chiefari, J.; Chong, Y. K.; Ercole, F.; Kristina, J.; Jeffery, J.; Le, T. P.; Mayadunne, R. T. A.; Meijs, G. F.; Moad, C. L.; Moad, G.; Rizzardo, E.; Thang, S. H. Macromolecules 1998, 31, 5559-5569.



일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: II-POLY.P-113

발표분야: 고분자화학

발표종류: 포스터, 발표일시: 목 15:00~17:00

Modification of Dye-sensitized Solar Cells Dye Surface using poly(quaternized *N*-Vinyl imidazole)-*co*-poly(*N*-Vinyl amine)

주창환, *이재준, 백현종

부산대 고분자공학과 *건국대 응용화학과

The dye-sensitized solar cells (DSSCs) has attractive features of high energy conversion and low production cost. The blocking layers play high efficiency in the photovoltaic process of the DSSCs. Poly(quaternized *N*-vinyl imidazole)-*co*-poly(*N*-vinyl phthalimide) (pQVIm-*co*-pNVPI) used in DSSCs was synthesized by reversible-addition fragmentation transfer (RAFT) polymerization. Poly(quaternized *N*-vinyl imidazole)-*co*-poly(*N*-vinyl amine) (pQVIm-*co*-pVAm) were prepared via hydrazinolysis reaction of pQVIm-*co*-pNVPI. The modified DSSC cells were prepared by carbodiimide-mediated coupling reaction of pQVIm-*co*-pVAm and N3 dye. The synthesized copolymers were characterized by FT-IR and ¹H-NMR spectroscopy. The modified DSSC cells were characterized by FT-IR, XPS to verify the amide bond. The DSSC performance using surface modification cells was 0.77 V, 8.69 mA/cm², 0.68 and 3.55 % under AM 1.5.

일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: II-POLY.P-114

발표분야: 고분자화학

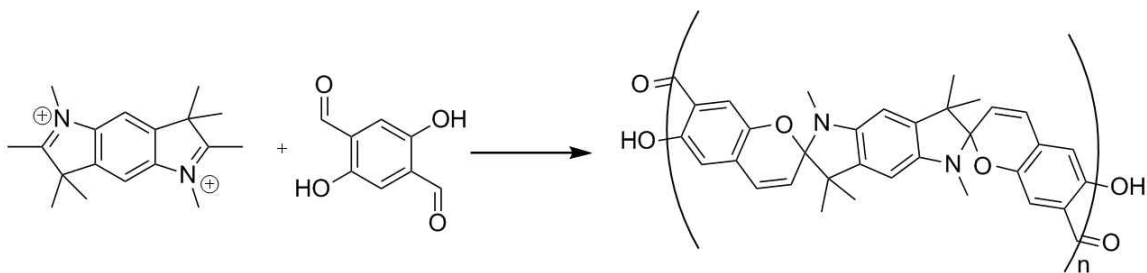
발표종류: 포스터, 발표일시: 목 15:00~17:00

Photoresponsive Poly(Spiropyran)

지승욱, 이성민, *강영종

한양대 화학과 *한양대 자연과학대학 화학과

Photoconductive organic materials have attracted intensive interests due to their potential applications in optoelectric devices, xerographic devices, sensors and so on. [1]-[2] Generally, photoconductive polymers are either conjugated polymers[3] or polymers containing chromophore in their main chain.[4] However, disadvantage of these systems is hard to optimize the intermolecular assembly to achieve high photoconductivity and photosensitive rate. Herein, we report synthesis and characterization of novel photoresponsive Poly(spiropyran). Spiropyran is a well known organic dye exhibiting significant changes in optical properties as well as molecular conformations upon irradiation of light. Photoresponsive Poly(spiropyran) shows increased conjugation length according to significant conformation changes with irradiation of light. The photoresponsive conformation and morphology changes and optical properties of Poly(spiropyran) will be characterized using SEM, TEM, PL and UV.[1] Che, Y.; Yang, X.; Liu, G.; Yu, C.; Ji, H.; Zuo, J.; Zhao, J.; Zang, L. J. Am. Chem. Soc. 2010, 132, 5743 [2] Zhang, X.; Jie, J.; Zhang, W.; Zhang, C.; Luo, L.; He, Z.; Zhang, X.; Zhang, W.; Lee, C.; Lee, S. Adv. Mater. 2008, 20, 2427[3] Jenekhe SA and Yi S, Adv Mater. 2000, 12, 1274 [4] Nakjoong Kim, Jin-Woo Oh, J. Mater. Chem., 2009, 19, 5765



일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: II-POLY.P-115

발표분야: 고분자화학

발표종류: 포스터, 발표일시: 목 15:00~17:00

A Planar Low Band Gap Copolymer for Photovoltaic Cells

이원호, *우한영

부산대 나노융합기술학과 *부산대 나노기술대학 나노정보소재공학과

A planar D-A type conjugated copolymer PTBT, which consists of alternating thiophene and alkoxy substituted benzothiadiazole, was synthesized by stille polycondensation. Our polymer is designed with two alkoxy chains which make the polymer soluble in organic solvents on the benzothiadiazole group resulting in the enhanced planarity and rigidity of the polymer. Moreover, a HOMO level was not increased because the HOMO is mainly related to the electron-rich moiety in the polymeric structure. The number-average molecular weight (Mn) was 30,000 g/mol by using gel permeation chromatography and optical band gap was 1.74 eV. The photovoltaic device characteristics will be discussed in detail.

일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: II-POLY.P-116

발표분야: 고분자화학

발표종류: 포스터, 발표일시: 목 15:00~17:00

Thermal properties of anionic copolymer : 2-pyrrolidinone with ϵ -caprolactam

선광민

한양대 유기나노공학과

Nylon is a synthetic fiber having the oldest history, and the polymer is connected by the amide bond. Among them, nylon4 is obtained by the ring opening polymerization of 2-pyrrolidinone, and it has advantages including the excellent modulus and high crease-resistance. But nylon4 has critical problem of low thermal decomposition temperature(T_d) which is lower than melting point(mp). In this study, 2-pyrrolidinone with ϵ -caprolactam copolymer was synthesized by anionic ring-opening polymerization and the thermal property was observed by DSC and TGA. The potassium tert-butoxide was used as an initiator and the benzoyl pyrrolidone was used as the activation reagent.

일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: II-POLY.P-117

발표분야: 고분자화학

발표종류: 포스터, 발표일시: 목 15:00~17:00

Copolymerization and Thermal Stability Analysis of Nylon 4

김선미, *조창기

한양대 유기나노공학과 *한양대 응용화학생명공학부

In this study, the synthesis and characterization of copolymers were investigated. The synthesis was performed by anionic ring-opening copolymerization of 2-pyrrolidinone. Sodium metal and potassium tert-butoxide were used as the catalysts and various activators were used. According to the copolymerization ratio with ϵ -caprolactam and a kind of activator, changes in molecular weight, melting temperature(mp), and thermal decomposition temperature(Td) were examined. Copolymer was analysed by FT-IR and H-NMR. Its molecular weight was obtained using intrinsic viscosity and its thermal properties were measured by TGA and DSC.

일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: II-POLY.P-118

발표분야: 고분자화학

발표종류: 포스터, 발표일시: 목 15:00~17:00

Correlation analysis of Nafion® properties and Humidity

송준섭, *조창기

한양대 유기나노 공학과 *한양대 응용화학생명공학부

Fuel cell is a device that directly converts chemical energy into electrical energy. Being positioned at between two catalytic electrodes, the membrane act as a pathway to deliver hydrogen ion from anode to cathode and also as isolation wall to prevent oxygen mixing with the fuel. Currently the Nafion® is used as a membrane in a fuel cell. Because Nafion® membrane shows superior physical and chemical properties. But Nafion® conductivity is sensitive to humidity. This study is the changes of Nafion® membrane properties with humidity relationship, also the connection between ion exchange capacity (IEC) and water uptake. Detailed results will be presented.

일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: II-POLY.P-119

발표분야: 고분자화학

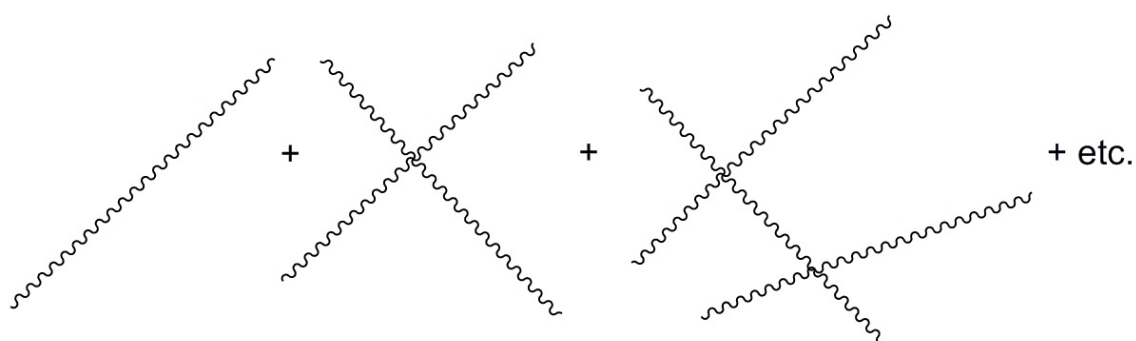
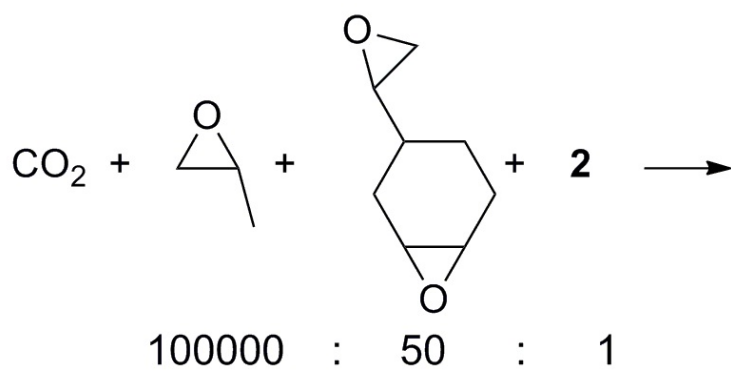
발표종류: 포스터, 발표일시: 목 15:00~17:00

CONNECTION OF POLYMER CHAINS USING DIEPOXIDE IN SYNTHESIS OF POLY PROPYLENE CARBONATE

KodiyamVarghese Jobi

아주대 분자과학기술학과

When a small amount of vinylcyclohexene dioxide ([diepoxide]/[cat] = 60, 0.14 w% propylene oxide) is additionally added in CO₂/propylene oxide copolymerization catalyzed by a highly active catalyst, cobalt(III) complex of a Salen-type ligand tethered by four quaternary ammonium salts (2), some polymer chains are connected consequently resulting in an increased molecular weight of up to Mw = 606000 and broadened molecular weight distribution. The same chain-connecting process is also applicable in the presence of chain transfer agent, tricarballic acid(C₃H₅(CO₂H)₃), 1,2,3,4-butanetetracarboxylic acid (C₄H₆(CO₂H)₄), or adipic acid (C₄H₈(CO₂H)₂), although a higher amount of diepoxide is needed. Gel permeation chromatography reveals multi-modal distributions along with a tail at a high molecular weight portion due to formation of the connected chains. The shape of the chain transfer agent varies the chain topology, but the rheological properties are not influenced by the topology change. The poly(propylene carbonate)-block-poly(ethylene glycol) copolymer, which is obtained by feeding poly(ethylene glycol)-OH as a chain transfer agent, becomes tough in the tensile properties and shows a high shear sensitivity in the rheological properties when some chains are connected using diepoxide.



~~~~~ = Poly(propylene carbonate)





일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: II-POLY.P-120

발표분야: 고분자화학

발표종류: 포스터, 발표일시: 목 15:00~17:00

## Crosslinked sulfonated polyimide copolymers for proton exchange membrane fuel cell (PEMFCs)

김주영, 권세진, \*이승우

영남대 화학공학과 \*영남대 디스플레이화학공학부

Proton exchange membrane fuel cells (PEMFCs) are considered as the most promising power source for automotive transportation in order to preserve oil resources and reduce significantly greenhouse gas emission. Most of them, sulfonated polyimides(SPIs) have been designed to be used as a proton conducting membrane in fuel cells. A series of SPIs containing were synthesized by two-step method polymerization. Material was prepared by the reaction of 4,4'-diaminodiphenyl ether-2,2'-disulfonic acid(ODADS), of p-phenylene diacric acid (PDA), p-phenylene diamine (PDA) and 4,4'-Oxydiphthalic anhydride (OPDA) in 1-Methyl-2-pyrrolidinone (NMP). The sulfonated monomer in the SPIs was varied from 0 to 50 wt %. The molecular structures of the SPIs were analyzed by means of fourier transform infrared spectrometer (FT-IR). Thermal Properties of the synthesized polymers were investigated by means of Thermogravimetric analysis(TGA) and Differential scanning calorimetry(DSC) . In addition, Ion exchange capacity(IEC) and Water Uptake(W.U) indicated high proton conductivity and excellent dimensional stability.

일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: II-IND.P-121

발표분야: 공업화학

발표종류: 포스터, 발표일시: 목 15:00~17:00

## Friction reduction properties of thiadiazole derivatives.

hoang quoc viet, 이신호, 김영준

충남대 화학과

Syntheses of novel dendrimers composed of glycerol, succinic acid with external thiadiazole groups are described. The 1st, 2nd and 3rd thiadiazole generations with 2, 4 and 8 thiadiazoles groups, respectively, were added to three different oil systems (1% wt): DB-51, Soybean and 100N. The friction reduction properties were measured by 4-ball WSD tester. Monothiadiazole derivatives were also synthesized and their friction values were compared with thiadiazole dendrimers.

일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: II-IND.P-122

발표분야: 공업화학

발표종류: 포스터, 발표일시: 목 15:00~17:00

## Diarylide pigment compositions for solvent-based gravure ink

박웅철, 이동훈

육성화학(주) 기술연구소

Typical surface treatment agents for diarylide pigments are amines and their results have increased tinctorial strength, gloss, transparency, and reduced rheology, but amine-treated pigments possess a major deficiency that exhibit poor storage stability and a red-to-green shift in hue, and also increase in viscosity. We investigated that diarylide pigment compositions useful for preparing storage stable and superior rheological printing ink (especially solvent-based gravure type) are prepared by reacting a primary amine-terminated alkylene oxide polymer substituted acetoacetanilide together with a typical acetoacetanilide and coupling the mixture of acetoacetanilides with tetrazotized dichlorobenzidine. In the present study, we have that the ink was 30% stronger color strength, more transparent and redder in hue than the prior art pigment composition. And also the ink exhibit significantly improved properties, particularly in providing lower rheology and dramatically improved storage stability.

일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: II-IND.P-123

발표분야: 공업화학

발표종류: 포스터, 발표일시: 목 15:00~17:00

## Practical hydrogen storage system based on dehydrogenation of ammonia borane for mobile application

김성관, 김태영, 강상욱

고려대 소재화학과

On-board hydrogen storage system with a 5.5 total system-wt% which enables a 300 mile driving range will be a milestone for the realization of a hydrogen economy. Various hydrogen storage materials have been proposed, and developed to meet the corresponding material based gravimetric target, 9 material weight percent  $H_2$  released (mat-wt%  $H_2$ ) which are mapped to the DOE (U.S. Department of Energy) technical targets. Among potential storage materials, ammonia borane ( $NH_3BH_3$ , AB) seems to be the most promising one by virtue of its high gravimetric hydrogen storage capacity, 19.6 wt%. To achieve the storage capacity over 9 mat-wt%  $H_2$ , AB solid or semi-solid state is suggested to be the best option and it will likely be necessary to develop heterogenous catalyst system to come along. Here, we report the tetraglyme (TG)-mediated, size-controlled synthesis of Palladium nanoparticles (PdNPs). Those PdNPs were easily redispersed in a minimum amount of TG with AB and shown to be highly active catalysts for AB dehydrogenation. During dehydrogenation, the spent fuels were mostly polyborazylene, which was an efficient solvent for further  $H_2$  dehydrogenation of AB. This advantageous solvent property of polyborazylene for AB minimized the use of TG. Most importantly, TG-mediated PdNPs were applied for the generation of  $H_2$  from AB/TG semi-solid state system, and recorded high hydrogen storage system {10.7 mat-wt %  $H_2$  [mat-wt %  $H_2 = H_2\text{-wt}/(AB+TG+PdNPs\text{-wts})$ ]} completing hydrogen release in 30 min at 85 °C. Such an unprecedented high hydrogen storage capacity comes from the synergistic effects facilitated by highly active PdNPs well-dispersed in TG medium and solvent property of polyborazylene.

일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: II-IND.P-124

발표분야: 공업화학

발표종류: 포스터, 발표일시: 목 15:00~17:00

## Practical hydrogen storage system based on dehydrogenation of metal hydride for mobile application: The effect of Pd nanoparticles on the decomposition of borohydrides in homogeneous solution

김성관, 김태영, 강상욱

고려대 소재화학과

Complex hydrides such as borohydrides ( $\text{BH}_4^-$ ) attracted considerable attention due to their high storage capacities. Among them,  $\text{LiBH}_4$  with a high theoretical storage capacity of 18.5 wt.% of  $\text{H}_2$ , has been considered as a good candidate for on-board applications. However, extraction of hydrogen from  $\text{LiBH}_4$  suffers due to the onset temperature of  $\text{LiBH}_4$  decomposition of ca. 400 °C and only half of the hydrogen being released below 600 °C. Consequently, recent research has focused on the catalyzed dehydrogenation of borohydrides ( $\text{BH}_4^-$ ) in order to lower the  $\text{H}_2$  evolution temperature and to increase the hydrogen desorption capacity. This is mainly due to the various complicated interactions involved in the solid state reactions in general: e.g. (a) chemical reactions of reactants and catalyst; (b) physical interactions in the solid state transformations, such as nucleation and growth, phase transformation and diffusion of molecules and atoms. In the present study we carried out the reactions under the homogeneous condition in solution phase. Tetraglyme (TG) was used as a solution matrix for homogeneous dehydrogenation because of its high boiling point (270 °C), the thermal stability and the solubility of borohydrides. We show the pressure change upon heating of  $\text{LiBH}_4$  solutions without additives. While the solid  $\text{LiBH}_4$  exhibits an decomposition at 450 °C, the onset temperatures of  $\text{LiBH}_4$  in TG are 250 °C. However, the molar ratio of released  $\text{H}_2$  to starting  $\text{LiBH}_4$  is about 3.4:1, which is larger than the nominal ratio (1.5:1). We attributed the excessive hydrogen to the side reaction of NaH or Al with the TG solvent. It is known that a transition metal species enhances the dehydrogenation of  $\text{LiBH}_4$  in solid state. We carried out the dehydrogenation in solution in order to examine if the palladium nanoparticles (PdNPs) enhances the reaction under homogeneous condition as in solid state. The results show that the PdNPs enhances the reaction in solution, the onset temperature of  $\text{LiBH}_4$  with PdNPs in TG

is 220 °C. One and two-dimensional solid-state  $^{11}\text{B}$ -NMR spectra of the  $\text{LiBH}_4$  spent fuel ( $\text{LiBH}_x$ ) sorted out all non-equivalent boron sites and classified them into  $\text{B}^3$  ( $\text{SP}^2$ ) and  $\text{B}^4$  ( $\text{SP}^3$ ) borons and the  $\text{SP}^2$  boron sites are rather similar to  $\text{SP}^2$  boron of B-O coordination. In addition, there are significant amount of organic species co-precipitated with  $\text{LiBH}_x$



일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: II-IND.P-125

발표분야: 공업화학

발표종류: 포스터, 발표일시: 목 15:00~17:00

## **Practical hydrogen storage system based on ammonia borane for mobile application: PdNPs-doped SBA-15 catalyst for dehydrogenation of ammonia borane**

김태영, 강상욱, 김성관

고려대 소재화학과

Well-dispersed palladium nanoparticles (PdNPs) in mesoporous SBA-15 were prepared in large quantity from a tetraglyme (TG) solution using an organopalladium precursor,  $\text{Pd}(\text{OAc})_6$ . Submicrometer-sized mesoporous silica SBA-15 with cuboidlike morphology has been prepared by using excess amounts of decane as cosolvent in the presence of  $\text{NH}_4\text{F}$ . The Pd/SBA-15 composites were characterized by X-ray diffraction (XRD), transmission electron microscopy (TEM), scanning electron microscopy (SEM), thermogravimetric analysis (TGA)/ Differential scanning calorimetry (DSC) and nitrogen adsorption analysis. XRD results indicate that as-synthesized nanocomposites basically remain ordered two-dimensional hexagonal mesostructure while TEM study exhibits a well dispersion of palladium nanoparticles within the mesoporous SBA-15 channels. The resulting Pd/SBA-15 nanocomposites were applied for dehydrogenation of ammonia borane.

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발표종류: 포스터, 발표일시: 목 15:00~17:00

## Development of Single-Site Catalyst for EPDM Polymerization: Synthesis and Structural Characterization of New Types of High Performance Half-Zirconocene Catalysts

이희준, 강상욱

고려대 소재화학과

Ligand effects on the catalytic activity [and propylene and ethylidene norbornene incorporation] for both ethylene polymerization and ethylene/propylene/ethylidene norbornene (EPDM) ter-polymerization using half-zirconocenes (zirconium half-sandwich complexes) containing 2-alkyl phenoxy ligand of type  $\text{Cp}^*\text{ZrCl}_2(2\text{-R-PhO})$  catalyst systems have been investigated.  $\text{Cp}^*\text{ZrCl}_2(2\text{-R-PhO})$  (R= Me 1, iPr 2, tBu 3, Ph 4) were prepared and identified by X-Ray crystal structure and  $^1\text{H}$  and  $^{13}\text{C}$  NMR spectra. The metal coordination geometry of each compound is best described as pseudo-tetrahedral, with the  $\text{Cp}^*$  ring and 2-R-PhO and chloride ligands occupying three leg positions in a piano-stool geometry. The catalytic activity for ethylene/propylene/ethylidene norbornene ter-polymerization increased in the order: 3 [22.7 Kg/(mmol of  $\text{Zr}\cdot\text{h}$ ), in toluene, ethylene 4 atm, 60 °C, 20 min, 44.55% C3 contents] > 2 [22.3 Kg/(mmol of  $\text{Zr}\cdot\text{h}$ ), in toluene, ethylene 4 atm, 60 °C, 20 min, 45.04% C3 contents] > 1 [18.3 Kg/(mmol of  $\text{Zr}\cdot\text{h}$ ), in toluene, ethylene 4 atm, 60 °C, 20 min, 42.08% C3 contents] > 4 [17.7 Kg/(mmol of  $\text{Zr}\cdot\text{h}$ ), in toluene, ethylene 4 atm, 60 °C, 20 min, 46.10% C3 contents], suggesting that a steric nature of the phenoxy ligand affects the activity. The phenoxy system showed the high catalytic activity for EPDM ter-polymerization with a unimodal molecular weight distribution and higher propylene incorporation.



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## Effect of Host Materials Hole Mobility in Single and co-Host EML Deep Blue PHOLEDs: Device Fabrication and Characterization of Carbazole Based Wide-Band-Gap Unipolar Host Materials

위경량, 강상욱

고려대 소재화학과

Since the pioneering report of Mark E. Thomson et al, phosphorescence light emitting devices (PHOLEDs) have attracted enormous interest for their 100 % internal quantum efficiency. In particular, efforts to achieve efficient deep blue PHOLEDs have led to considerable advances in materials chemistry. As a result, highly efficient wide band gap carbazole based unipolar host and Ir based dopant materials have been reported by many groups. Moreover, to achieve more efficient host materials, recent developments for host often focus on the synthesis of bipolar materials. However, in spite of advanced development in hosts, understanding the relationship between the hole mobility of host and device performance is important for successful development of deep blue PHOLEDs. In this study, six different p-type unipolar host materials (CzSi, CDBP, mCP, AK11, AK12, AK13) was presented and various hole mobility property in the range of  $10^{-5}$  ~  $10^{-3}$  cm<sup>2</sup> V<sup>-1</sup> s<sup>-1</sup> was examined by means of time of flight method. All unipolar carbazole materials were applied to Fir6 doped PHOLED device as a p-type co-host materials. In the co-host system, high hole mobility material (AK13) was showed high power efficiency (24 lm/W), high current efficiency (30 cd/A), and low turn-on voltages (3.4 V), while all host materials showed similar device performance (15 lm/W) in single host system.

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## **Development of highly efficient wide band-gap electron transporting materials for deep blue PHOLEDs: synthesis and photophysical properties of electron deficient heterocycles substituted dimethylsilane derivatives**

김애리, 위경량, 강상욱

고려대 소재화학과

In spite of the successful development of Firpic-based PHOLED, there are urgent needs for development of efficient deeper blue light emitting devices. However, to use deeper emitters such as Fir6 ( $ET = 2.82$  eV), not only wide band gap host material, but also higher band gap HTL and ETL materials should be introduced. As a consequence, development of wide band gap ( $T_1 > 2.9$  eV) host, HTL, and ETL materials has been a subject of interest. Recently, a number of promising host materials were reported, but wide band gap HTL and ETL materials with high charge mobility are still required for efficient deep blue PHOLED. In this study, to obtain wide energy gap ETL materials with high thermal stability, we carefully designed three different type of hetero aromatic building block substituted silane compounds, bis(4-(5-phenyl-1,3,4-oxadiazol-2-yl)phenyl)dimethylsilane (AK22), bis(4-(4,6-diphenyl-1,3,5-triazin-2-yl)phenyl)dimethylsilane (AK23), and bis(4-(1-phenyl-1H-benzoimidazol-2-yl)phenyl)dimethylsilane (AK24). All materials were prepared by direct substitution reaction between 2 equiv of lithium reagent and dichlorodimethylsilane in moderate yield. All silane based ETL materials were characterized regarding their optical and thermal properties. Different substitution patterns resulted in high glass-transition temperatures ( $T_g$ ) of up to 80 oC and triplet energies ( $\Delta E(T_1-S_0)$ ) of up to 2.95 eV. The application as ETL material for the blue phosphor iridium(III)[bis(4,6-difluorophenyl)-pyridinato-N,C2']tetrakis(1-pyrazolyl) borate (Fir6) yielded maximum current efficiencies up to 25 cd/A.

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## Effects of Ionic Periphery Group in Ruthenium-Complex-Sensitized TiO<sub>2</sub> Under Visible Light for DSSCs

정동철, 위경량, 강상욱

고려대 소재화학과

The conversion efficiency of dye-sensitized solar cells (DSSCs) has currently been improved to above 12%. However, due to the encapsulation problem posed by the use of the liquid electrolyte in conventional liquid electrolyte based DSSCs, solvent leakage and evaporation are two main challenges; therefore, much work is being done to make an all solid-state DSSC. In addition, the use of solvent free electrolytes in the DSSC is expected to offer stable performance for the device. In this study, an effort to develop of efficient Ru sensitizers for solid-state DSSC, we carefully designed and synthesized ionic periphery group substituted Ru sensitizers (Ru(NCS)<sub>2</sub>LX), where X and L consists of 4,4'-di(2,5,8,11-tetraoxadodecyl-1,3-dimethyl-1H-imidazol-3-ium)-2,2'-bipyridine and 2,2'-bipyridine-4,4'-dicarboxylic acid, respectively. Indeed, the ionic periphery group and bulkiness of the substituted ligand X induced molecular orientations and reduced aggregations on the TiO<sub>2</sub> surface.

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발표종류: 포스터, 발표일시: 목 15:00~17:00

## Structure-Activity Correlation in Half-titanium Single-Site Olefin Polymerization Catalysts Containing Electronic Alteration at 2-Phenyl Group and 4-Position of the Phenoxy Ligation

김태진, 김성관, 한원식, 이희준, 강상욱

고려대 소재화학과

A series of 2-phenyl phenoxy ligands of Type I-III was synthesized, varying with a wide range of electron-donating and -withdrawing substituents either at the 4-position of the 2-phenylphenoxy ligand or 2' and 4' positions of the 2-position phenyl substituent to investigate electronic effects at the titanium metal center of the half-titanocene dichlorides with Cp\* ancillary ligand. Electronic alteration was focused at the three different sites on 2-phenyl phenoxy ligand, one at the 2-position phenyl group (Type II) and the other two at the 4-position with a direct substitution (Type I) or substitution through another phenyl ring (Type III). This resulted in a wide variety of electronically tuned titanium complexes comprised of 2-Ph-4-X-PhO (Type I, X = F, 5a; Cl, 5b; Me, 5c; Pri, 5d; But, 5e; OMe, 5f), 2-(4'-X-Ph)-PhO (Type II, X = CF<sub>3</sub>, 10a; F, 10c; OMe, 10d) and 2-(2',4'-F<sub>2</sub>-Ph)-PhO 10b, and bridging phenyl substituents, 2-Ph-4-(2',4'-F<sub>2</sub>-Ph)PhO 13a and 2-Ph-4-(4'-X-Ph)PhO (Type III, X = F, 13b; Cl, 13c; H, 13d; But, 13e; NMe<sub>2</sub>, 13f). In Type I, a systematic electronic perturbation was confirmed by Hammett plot of the para substituents ( $\sigma_p$ ) with respect to the reduction potential at the titanium metal. Substitution with electron-donating or -withdrawing groups at the phenoxy ligand allowed electronic alteration at the titanium metal center to give a direct structure-activity relationship. As catalysts for ethylene homopolymerization at high temperature (140 °C), para- and ortho- substituted Type I and Type II showed higher activities than that of Type III on the basis of initial enthalpy change of polymerization. Further, in general 2-phenylphenoxy system with electron-withdrawing groups showed superior activities to with electron-withdrawing groups and in each system fluorine substitution gave rise to the best activity with 37.2, 34.2, and 43.2 Kg/(mmol of Ti•h) for 5a, 10a, and 13a, respectively. As the substituent becomes more electrons withdrawing, higher molecular weight was obtained: In the case of 5a, Mw= 372,000

exceeded over to the value of  $M_w = 222,000$  for 5f. In particular, 5a exhibited the ethylene copolymerization catalytic activity of 39.0 Kg/(mmol of  $Ti\bullet h$ ) with 1-octene, surpassing the reference catalyst  $Cp^*Ti(2-Ph-PhO)Cl_2$  of 34.2 Kg/(mmol of  $Ti\bullet h$ ).



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발표종류: 포스터, 발표일시: 목 15:00~17:00

## Development of a Wide Band-gap Bipolar Host Material for Blue Phosphorescent OLEDs: Synthesis and Characterization of Silicone Cored Carbazole/Triazole Hybrid Molecule

정소영, 김애리, 위경량, 강상욱

고려대 소재화학과

To achieve a highly efficient phosphorescent OLED, a triplet emitter is normally doped into a host material to reduce concentration quenching. It is essential that the triplet energy of the host is higher than that of the emitter in order to prevent energy back transfer from the phosphorescent guest to the host. This becomes more challenging for host materials used in combination with blue phosphorescent emitters, where triplet energies larger than 2.8 eV are required. Recent developments of new matrix materials for phosphorescent organic light-emitting diodes often focus on the synthesis of bipolar materials. In this report, to achieve a wide band-gap bipolar host material with high thermal stability, a silicon atom was introduced between 4-(N-carbazolyl)phenyl (p-type) and 3,4,5-triphenyl-1,2,4-triazole (n-type) molecules. As a result, [(4-(4,5-diphenyl-4H-1,2,4-triazol-3-yl)phenyl)(4-(carbazol-9-yl)phenyl)]dimethylsilane (AK41) was prepared by direct substitution reaction with dimethyldichlorosilane. AK41 showed high triplet energy of 2.9 eV and high glass transition temperature of 91 °C. By employing AK41 as a bipolar host material of iridium(III)[bis(4,6-difluorophenyl)pyridinato-N,C2']tetrakis(1-pyrazolyl)borate (FIr6) based deep blue phosphorescent OLEDs, a maximum external quantum efficiency (EQE) of 14%, and deep blue color coordinates of (0.15, 0.22) were achieved.

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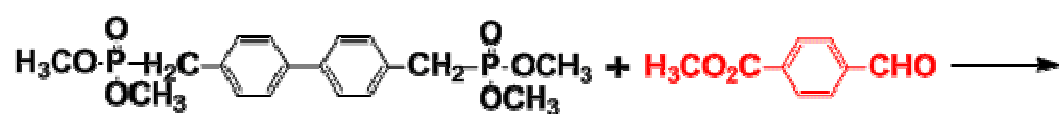
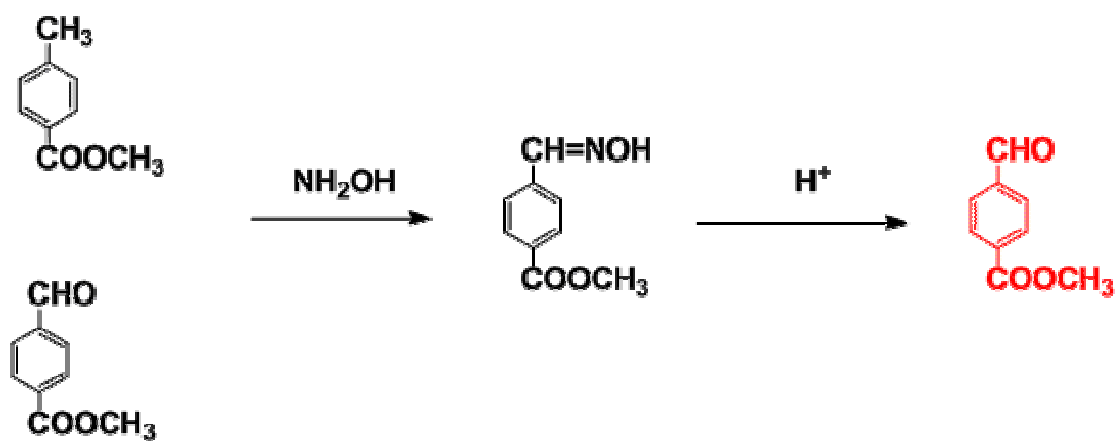
발표종류: 포스터, 발표일시: 목 15:00~17:00

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

이윤아, 유영, 김기림, 김석찬

국민대 화학과

PET의 원료가 되는 dimethylterephthalate (DMT)는 *p*-xylene의 산화과정을 통해 만들어진다. 이 과정에서 부산물로 methylformylbenzoate (MFB)가 생성된다. MFB는 자체의 악취와 폐기처리의 어려움이 있고, 폐기 과정에서 과량의 CO<sub>2</sub>를 발생시킨다. 이 MFB를 활용하기 위하여 mixture MFB를 hydroxylamine salt와 합성시켜 순수한 MHB를 얻어낸 뒤, MHB를 환원시켜 고순도 MFB를 얻어낸다. 이 MFB를 tetramethyl biphenyl-4,4'-diylbis(methylene)diphosphonate와 Wittig reaction하여 conjugation된 형광증백제 MFB-F를 합성하였다. 또한 MFB의 다양한 유도체를 만들어 여러종류의 형광증백제를 합성함으로써, 산업폐기물을 활용한 고부가 가치를 합성하였다.





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발표종류: 포스터, 발표일시: 목 15:00~17:00

## Photocatalytic Hydrogen Production from Water Catalyzed by Polypyridyl Iridium(III)–Platinum(II) Heterobinuclear Complexes with High Quantum yield

변성민, 한원식, 김현영, 강상욱

고려대 소재화학과

Three heterobinuclear complexes  $[(dfppy)_2Ir(dpp)PtCl_2]$ ,  $[(ppy)_2Ir(dpp)PtCl_2]$ , and  $[(btp)_2Ir(dpp)PtCl_2]$  (where  $dfppy$  = 2-(4,6-difluoro-phenyl)pyridine,  $ppy$  = 2-phenylpyridine,  $btp$  = 2-phenylbenzo[d]thiazole, and  $dpp$  = 2,3-bis(2-pyridyl)pyrazine) were prepared, in which the polypyridyl iridium photosensitizer and the platinum catalyst are connected by bridging ligand. The emission intensity of heterobinuclear complexes are much smaller than those of corresponding mononuclear complexes, indicating that platination of a precursor complexes results in quantitative quenching of the  $^3MLCT$  emission from the  $L_2Ir^*(dpp)_2^+$  moiety which attributed to intramolecular electron transfer to give  $Ir(d\pi) \rightarrow Pt(d\sigma^*)$  CT excited state ( $^3MMCT$ ). The photochemical hydrogen evolution from water driven by prepared heterobinuclear complexes in the presence a sacrificial electron donor (TEOA) was investigated. The intramolecular energy transfer followed by electron transfer in Ir(III)–Pt(II) based molecular photocatalysts can be occur efficiently, which leads to control of the photohydrogen-evolving activity of these molecular photocatalysts.

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## Photoinduced Hydrogen Evolution Catalyzed by Iridium(III)– Platinum(II) Heterobinuclear Dendrimers with Carbazole Dendron as a Light-Harvesting Antenna

김현영, 한원식, 변성민, 강상욱

고려대 소재화학과

In an effort to develop an efficient photocatalytic system for hydrogen evolution, Ir(III)-Pt(II) heterobinuclear dendrimers, (dfppy-Cz<sub>n</sub>)<sub>2</sub>Ir(dpp)Pt and (dfppy-Cz<sub>n</sub>)<sub>2</sub>Ir(tpphz)Pt, and its parent mononuclear dendrimers, (dfppy-Cz<sub>n</sub>)<sub>2</sub>Ir(dpp) and (dfppy-Cz<sub>n</sub>)<sub>2</sub>Ir(tpphz), were prepared where Cz<sub>n</sub> (n=0, 1, 2) is phenylcarbazole dendrons. In mononuclear dendrimers, PET process from the light-harvesting dendrons to the Ir-core revealed by the steady-state and time-resolved spectroscopic measurements. The results showed that Ir(dfppy-Cz<sub>n</sub>)<sub>2</sub>L (L = dpp and tpphz) dendrimers undergo the electron transfer in an efficiency of >90% from Cz to the core, especially to dpp and thhpz ligand for all homonuclear dendrimers. The photochemical hydrogen evolution from water driven by heterobinuclear dendrimers in the presence a sacrificial electron donor (TEOA) was investigated. Among the dendrimers, 1st-generation dendrimers showed higher hydrogen evolution efficiency compared to that of 2nd-generation dendrimer, probably due to the shorter distance between Cz and the Ir-core which facilitate energy transfer.

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## Hydrophilic-Substituent Effect on Organic Dye Sensitized Water Splitting Photocatalyst in Visible-Light: Substituent Dependent Charge Recombination and Dye Regeneration in the Presence of Sacrificial Reagent

한원식, 김현영, 변성민, 강상욱

고려대 소재화학과

A series of hydrophobic, slightly hydrophilic, and hydrophilic dyes were synthesized and applied to sensitized hydrogen generation based on Pt/TiO<sub>2</sub>/Dye photocatalysts. The hydrophilic photocatalysts showed substantially higher H<sub>2</sub>- generation efficiencies than the hydrophobic photocatalyst. Rise behavior of the radical cation of the dye and conduction-band-electron is studied by femtosecond transient absorption measurements in the visible and NIR regions, and results showed that the electron injection for both hydrophobic and hydrophilic dye is ultrafast in picosecond range. This should correspond to an electron injection efficiency of 100% for both dyes, as the fluorescence lifetime is at least 3 orders of magnitude longer than the injection. Rather, the hydrogen generation efficiency-limiting step seems to be components of fast charge recombination between the electrons injected into the TiO<sub>2</sub> and the oxidized dye. In the cases of hydrophilic dye, ethylene-oxide chains make the dye surface miscible with the aqueous phase so that charge recombination was impeded and dye regeneration was facilitated by approaching of sacrificial reagent close to the radical cation center.

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## **Separation method of bio-process succinate salt from using enzyme (Novozyme 435) in organic solvent–water system**

이병욱, 김영준

충남대 화학과

The technologies using fermentation broth can be used to manufacture high quality products for environment, energy and fine chemistry. We synthesized valuable dialkylsuccinate using succinate salt (82.3g/L) obtained from bioprocess with alcohol in organic solvent-water biphasic system. The product of this reaction was separated easily through a simple filtration step that allows removing water soluble byproducts. In this experiment, enzyme (Novozyme 435) was used as a catalyst and it was very sensitive to acid condition. The yield of product was the highest at about pH 1.5~3 and purity was higher than 90 %.

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## Effect of ketimide ligand for ethylene polymerization and ethylene/propylene/norbornene ter-polymerization catalyzed by (cyclopentadienyl)(ketimide)titanium complexes-MAO catalyst systems

정재호, 김태진, 이희준, 강상욱

고려대 소재화학과

Ligand effects on the catalytic for ethylene polymerization and ethylene/propylene/norbornene ter-polymerization using half-titanocenes (titanium half-sandwich complexes) containing ketimide ligand of type  $\text{Cp}^{\wedge}\text{TiCl}_2[\text{N}=\text{C}(\text{Ar})_2]$  [ $\text{Cp}^{\wedge} = \text{Cp}$  (1),  $\text{C}_5\text{Me}_5$  (2);  $\text{Ar} = 2\text{-isopropylphenyl}$  (a),  $2,6\text{-diisopropylphenyl}$  (b), imidazole (c)],  $\text{Cp}^{\wedge}\text{TiCl}_2(\text{L})$  [ $\text{L} = 1,3\text{-bis}(2,6\text{-diisopropylphenyl})\text{-1H-imidazol-2(3H)-imine}$  (d),  $1,3\text{-diisopropyl-1H-imidazol-2(3H)-imine}$  (e)]-methylaluminoxane (MAO) catalyst systems have been investigated. It has been revealed that these complex catalysts displayed unique characteristics especially for ethylene (ter) polymerizations and some examples are known to produce new polyolefins that cannot be prepared by ordinary catalysts such as classical Ziegler-Natta, metallocenes. Modification of both cyclopentadienyl fragment and anionic ancillary donor ligands are the key for precise olefin (ter)polymerization.

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## High molar extinction coefficient organic sensitizers for dye sensitized solar cell based on TiO<sub>2</sub> particles under visible light

조양진, 위경량, 강상욱

고려대 소재화학과

Considerable attention has been paid to semiconductor TiO<sub>2</sub> in connection to the creation of clean energy, typically hydrogen evolution from water and electricity generation by solar cells under solar-light illumination. Due to little visible-light absorption by TiO<sub>2</sub>, dye modification has been used to make TiO<sub>2</sub> active to visible-light excitation, typically in dye-sensitized solar cell using TiO<sub>2</sub> particles. In this study, a series of thiophene-vinyl-thiophene linker substituted organic dye, (E)-2-cyano-3-(5-((E)-2-(5-(4-(diphenylamino)phenyl)thiophen-2-yl)vinyl)thiophen-2-yl)acrylic acid, where diphenylamino was varied from -H (1) and -CH<sub>2</sub>OCH<sub>3</sub> (2) at the 4-position of phenyl, was successfully prepared. The maximum UV/Vis absorption of 1 and 2 showed 472 and 477 nm, respectively, with high molar extinction coefficient ( , M<sup>-1</sup>cm<sup>-1</sup>= 81,000). The solar-cell performance of DSSCs based on dye-grafted nanocrystalline TiO<sub>2</sub> using 1, 2, and standard N3 were compared, revealing substantial dependences on the dye structures, particularly on the -OMe substituent.

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발표종류: 포스터, 발표일시: 목 15:00~17:00

## Ether-functionalized ionic liquids as highly efficient SO<sub>2</sub> absorbents

홍성윤, 이지선, 정민석, 김훈식

경희대 화학과

Room temperature ionic liquids (RTILs), ether-functionalized imidazolium methane sulfonates 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 methane sulfonate 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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발표종류: 포스터, 발표일시: 목 15:00~17:00

## Application of ionic liquids to electrolytes for lithium batteries

임진균, 전영은, 정민석, 김훈식

경희대 화학과

The development of advanced materials for energy storage and conversion has been receiving wide attention to meet the rising demand of clean energy technologies. The cathodic stability of the zwitterionic imidazolium compounds was significantly enhanced by the introduction of an ether group at 1 or 2-position on the imidazolium ring. The cycle performance tests showed that the initial cell capacity was maintained almost unchanged up to 100 cycles at 0.5 and 1 C when 2.5 wt.% of 2-butoxymethyl-1-methylimidazolium-3-propylsulfonate or 2-butoxymethyl-10butylimidazolium-3-propylsulfonate was added to the model electrolyte (1 M LiPF<sub>6</sub> in ethylene carbonate, dimethyl carbonate and ethylmethyl carbonate (1/1/1 v/v/v)). Structures of zwitterionic compounds and their interactions with lithium ions were theoretically investigated.



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발표종류: 포스터, 발표일시: 목 15:00~17:00

## Comparative Energy and Electron Transfer via Dendritic Generation of the Phosphorescent Metal Iridium Complexes

황아름, 조대원, \*강상욱

고려대 신소재화학과 \*고려대 소재화학과

Light-harvesting systems based on phosphorescent dendrimers ( $\text{Ir}(\text{dfppy})_2\text{-Czn}$  and  $\text{Ir}(\text{ppy})_2\text{-Czn}$ ,  $n = 1, 2, 3$ ) with an iridium complex core (iridium(III) bis[(4,6-difluorophenyl)pyridinato-N,C2]-3-hydroxypicolinate derivative and iridium(III) bis(phenylpyridinato-N,C2)-3-hydroxypicolinate derivative) and phenyl carbazole dendrons were prepared and their photophysical properties were investigated. The light-harvesting ability of Ir dendrimers increases with the generation due to an increase of the number of phenyl carbazole units. The efficiencies for energy transfer from carbazole units to Ir core in  $\text{Ir}(\text{dfppy})_2\text{-Czn}$  are 98, 95 and 92% for generations 1–3, respectively. For  $\text{Ir}(\text{ppy})_2\text{-Czn}$  ( $n = 1, 2, 3$ ), energy transfer efficiencies and the rate constants are 98, 95 and 90% for generations 1–3, respectively. Moreover, the transient absorption spectra of Ir dendrimers show the formation of the Cz cation radical species generated by photoinduced electron transfer (PET) at 800 nm. Consequently, these dendrimer systems can provide unique functions such as “antenna effect” and “photoinduced charge separation”.

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발표분야: 공업화학

발표종류: 포스터, 발표일시: 목 15:00~17:00

## **Enhanced metal-free membranes for the separation of CO<sub>2</sub>/CH<sub>4</sub> mixtures: Imidazolium-based Room-Temperature ionic liquids as CO<sub>2</sub> transport carriers**

이진규, 김영진, 정민석, 김훈식

경희대 화학과

Imidazolium-based ionic liquids with a basic anion were shown to be highly effective carbon dioxide transport carriers for the selective separation of carbon dioxide in methane through membranes. The highest selectivity of 45 was attained when 1-octaethylene glycol monomethyl ether-3-methylimidazolium methanesulfonate was used as the transport carrier.

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발표분야: 공업화학

발표종류: 포스터, 발표일시: 목 15:00~17:00

## Preparation of conductive water-borne polyurethane dispersion

박상하

조선대 화학과

PU(polyurethane) can be used as a good material in various industrial fields, such as durable elastomeric wheels and tires, spandex fibers, high performance adhesives and sealants. However, polyurethane traditionally has been manufactured using organic solvents, such as Benzene, Toluene, Xylene(BTX). Due to the problem that the process of producing organic solvent can cause many environmental problems, and VOC(volatile organic compound) regulations are also increasingly expanding. Therefore, the studies on using water as the solvent instead of the BTX and improving variable properties of water-borne polyurethane dispersion(WPU) have been attracted a lot of attentions recently. In this study, the polyurethane prepolymer was prepared from polyol, isophrone diisocyanate(IPDI), and dimethylol propionic acid(DMPA). Then, aniline was capped on the NCO group of the prepolymer. Finally, we blended CNT(carbon nano tube) with WPU to give anti-static properties. The aniline terminated WPU showed better conducting properties than pure WPU when CNT was blended. We also examined changes of other properties due to the addition, such as coating membrane's transmittance, adhesion, and pencil hardness.

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발표종류: 포스터, 발표일시: 목 15:00~17:00

## **Ionic liquids as benign catalysts for the carbonylation of amines to formamides**

최영섭, \*이제승, \*김훈식, 장호겸

고려대 화학과 \*경희대 화학과

1-Butyl-3-methylimidazolium hydrogen carbonate ([BMIm]HCO<sub>3</sub>), prepared from the reaction of [BMIm]Cl with K<sub>2</sub>CO<sub>3</sub> in methanol, exhibited much higher activity than other ([BMIm]-based ionic liquids for the carbonylation of amines to manufacture formamides. The computational calculation results on the carbonylation reaction of methylamine implies that the higher activity of [BMIm]HCO<sub>3</sub> could be ascribed to the bifunctional actions as a hydrogen atom acceptor and a donor.

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발표분야: 공업화학

발표종류: 포스터, 발표일시: 목 15:00~17:00

## Utilization of CO<sub>2</sub> in carboxylation of amine catalyzed by Ionic liquids

심유나, 김진형, 정민석, 김훈식

경희대 화학과

Carbon dioxide is very abundant carbonyl resource. But because of the ability causing greenhouse effect, the utilization of carbon dioxide to useful materials is important process. Especially 1,3-disubstituted ureas have an important role in variable application and organic synthesis as a carbonyl compound. We could synthesize the 1,3-disubstituted ureas from the carboxylation of amines by CO<sub>2</sub> and ionic liquid was used as catalyst. And we discovered that ionic liquid, especially [BMIM]Cl behave as a powerful catalyst for the reaction between primary amines and CO<sub>2</sub>

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발표분야: 공업화학

발표종류: 포스터, 발표일시: 목 15:00~17:00

## Anti-fouling and water resistance properties of SPC resins containing OSE polymers

최은윤, \*박 현

부산대 조선해양공학과 \*부산대 첨단조선공학연구센터

The self-polishing copolymer(SPC)s prevent the adhesion and the growth of microorganisms, animals and plants in the sea, it is called biofouling, on the ships because SPCs reacts with the salt in the sea and are constantly eroded. So it has been variously applied to antifouling paints as the binder. Currently Tin-free and Copper-free SPC paints have been actively developed to solve environmental problems. There were researches that the biofouling phenonena was hindered on the surface which has its surface energy between 20 and 30(mN/m). The representative material for the low surface energy is the Poly[oxy(n-octylsulfonylmethyl)ethylene](OSE). In this study we synthesized OSE and two kinds of Zn-based copolymer by using the Zinc methacrylate(ZMA) and Styrene or Butyl acrylate to find out anti-fouling and abrasion resistance properties. The structures of the synthesized polymers were confirmed using  $^1\text{H}$ -NMR and FT-IR. Other properties of samples are investigated through the immersion and abrasion resistance tests at the static state. Even though the results did not show the direct correlation between the contents of OSE and antifouling performance, the contents of OSE influenced properties of abrasion resistance of SPCs.

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발표분야: 공업화학

발표종류: 포스터, 발표일시: 목 15:00~17:00

## 실리콘오일을 이용한 UV경화형 폴리우레탄 발수제 제조

이채호, \*박관희, \*조석준, \*\*이종대, \*\*\*강상욱

원광대 생명나노화학부 \*원광대 화학과 \*\*조선대 화학과 \*\*\*고려대 소재화학과

물과의 접촉각이 높은 발수성 코팅 도료는 터치용 핸드폰, 자동차외장과 섬유등의 많은 산업 분야에서 활용되고 있다. 기존의 발수제는 불소계열 제품이 많이 상용화 되어있지만 높은 가격의 문제점을 보완하기 위하여 가격이 저렴한 실리콘오일을 이용하여 발수성을 부여하는 연구가 활발히 이루어지고 있다. 실리콘오일은 전단저항성, 낮은 증기압, 낮은 표면장력, 뛰어난 전기특성, 발수성, 소포성, 이형성 등의 장점을 가지고 있는데 이러한 실리콘오일만으로는 기계적 물성과 성형성 등의 기능을 부여할수 없는 실정이다. 본 연구에서는 기존의 발수성 제품의 단점을 보완하기 위하여 polyol 과 isocyanate 를 반응시켜 organic solvent-based polyurethane 을 제조하였다. 이 때 NCO group 에 발수성 기능을 내포한 silicon oil 을 capping 시킨 후 광 개시제를 첨가하여 UV 경화함으로서 코팅 막의 내구성을 증진시킨 발수성 하드코팅막을 제조하였다.

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발표분야: 공업화학

발표종류: 포스터, 발표일시: 목 15:00~17:00

## Structural and catalytic properties of Titania supported Antimony-Vanadia catalysts for NH<sub>3</sub>-SCR

이경주, \*하현필

고려대 화공생명공학과 \*KIST 기능재료센터

To get the high efficiency NO<sub>x</sub> conversion controlled state of titania (slurry and powder) supported antimony-vanadia catalysts in the reduction of nitrogen oxides (NO<sub>x</sub>) by NH<sub>3</sub> through selective catalytic reduction (SCR) study was carried out. Controlled state of TiO<sub>2</sub> catalysts were prepared by impregnation method and characterized by X-ray diffraction (XRD) and Brunner Emmett Teller surface area (BET-SA). In situ electrical conductivity and X-ray photoelectron spectroscopy (XPS) measurement was carried out for Sb(2%)/V<sub>2</sub>O<sub>5</sub>/TiO<sub>2</sub> and compared with commercial TiO<sub>2</sub>. Both powder TiO<sub>2</sub> and slurry TiO<sub>2</sub> supported Sb-V<sub>2</sub>O<sub>5</sub> catalysts showed high catalytic activity for NH<sub>3</sub> selective catalytic reduction (NH<sub>3</sub>-SCR) of NO<sub>x</sub> carried at temperatures between 300 and 400°C.



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발표분야: 공업화학

발표종류: 포스터, 발표일시: 목 15:00~17:00

## The Effect of Mg Addition on the Selective Catalytic Reduction of NO<sub>x</sub> with CH<sub>4</sub> on Ag/Al<sub>2</sub>O<sub>3</sub> Catalysts

유창용, 하헌필, 배현숙, \*K.Narayana Rao

KIST 기능재료센터 \*Indian Institute of Chemical Technology

The influence of sulfate on the selective catalytic reduction of NO<sub>x</sub> on the Ag/Al<sub>2</sub>O<sub>3</sub> catalyst was studied when CH<sub>4</sub> was used as a reducing agent. Various preparation methods influenced differently on the de NO<sub>x</sub> activity. Among the methods, cogelation precipitation gave best activity. When sulfates were formed on the surfaces of samples prepared by impregnated and deposition precipitation, de NO<sub>x</sub> activity was enhanced as long as suitable forming condition is satisfied. The major sulfate formed in Ag/Al<sub>2</sub>O<sub>3</sub> catalyst was the aluminum sulfate and it seems that this sulfate acted as a promoter. When Mg was added to the Ag/Al<sub>2</sub>O<sub>3</sub> catalyst it promoted de NO<sub>x</sub> activity at high temperature. Intentionally added sulfate also enhanced de NO<sub>x</sub> activity, when their amount was confined less than 3wt%.

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발표종류: 포스터, 발표일시: 목 15:00~17:00

## Convenient synthesis of a series of dicyclopentadiene derivatives as new candidates for synthetic lubricants

김남균, \*최진일, \*\*정근우

한국화학연구원 \*한국화학연구원 에너지소재 \*\*한국화학연구원 응용화학연구단

A series of cyclopentadiene (CPD) based synthetic base oils were prepared by dicyclopentadiene (DCPD) which obtained as a by-product of naptha cracking process. The CPD based synthetic oils were prepared by 3 steps include alkylation of CPD with several alcohols in the presence of KOH as a base, Diels-Alder reaction of alkylated CPD with maleic anhydride, and esterification of Diels-Alder adducts with several alcohols. The structures of synthesized ester derivatives were characterized through <sup>1</sup>H-NMR, FT-IR, and GC/MS analyses. Also, physical properties such as kinematic viscosity, pour point, density, and refractive index were evaluated and the properties depended on the number of alkyl chain with CPD and the type of alkyl group of esters.

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발표종류: 포스터, 발표일시: 목 15:00~17:00

## 새로운 TAED 합성 방법

심주용, 유국현, 서용성

동국대 화학과

TAED (Tetraacetylenediamine)는 세탁표백제의 저온 활성을 유도하는 촉매제로 분말세제원료의 핵심 소재이다. 이 물질은 acetic acid와 ethylenediamine의 1차 합성결과물인 DAED (Diacetylenediamine)을 이용하여 무수초산과 2차 반응을 통해 TAED를 얻는다. 하지만 2단계 반응은 수율이 30%이하로 극히 낮아 산업적 상용화를 위해 정량비의 2배 이상의 과량의 무수초산을 사용하여 60% 수율을 얻고 있다. 따라서 과량의 무수초산으로 인해 야기되는 환경오염 및 과량 원료사용에 따른 비용문제가 이슈화 되고 있다. 본 연구는 현재 TAED 생산의 문제점들을 보완하고 고수율의 합성 수율을 낼 수 있는 새로운 합성방법에 대한 연구를 추진하였다. 이를 통해 기존합성에서 과량 사용되는 무수초산의 사용량을 당량비인 1:2 합성비로 개선하여 오염물질 배출을 최소화 할 수 있으며 합성 후 얻어지는 TAED의 수율을 획기적으로 개선할 수 있음을 확인 하였다.

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발표종류: 포스터, 발표일시: 목 15:00~17:00

## Modification of Spherical Silica Particles with a Silanepolyol and Its Characterizations

이중석, 한준수, 유복렬

KIST 나노재료센터

Much attention has been paid to the surface modification of inorganic particles to have a hydrophobic property on its surface that can be applicable to a polymer composite. We have been evaluating the silanepolyols as a modifier instead of alkoxysilane, which is widely used. In this study, spherical silica ( $230\pm30$  nm) was prepared and modified with a silanepolyol,  $\text{PhSi}(\text{OH})_3$ , in a wide range from 0.1 to 10 wt % based on the silica used. Characterizations of the modified particles were carried out using various analytical tools (SEM, TEM, DLS, etc.). Herein, recent results for the surface modification approach to silica and several inorganic particles ( $\text{TiO}_2$ ,  $\text{SnO}_2$ ,  $\text{ZnO}$ ) including their detailed analytical results will be discussed.

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발표분야: 공업화학

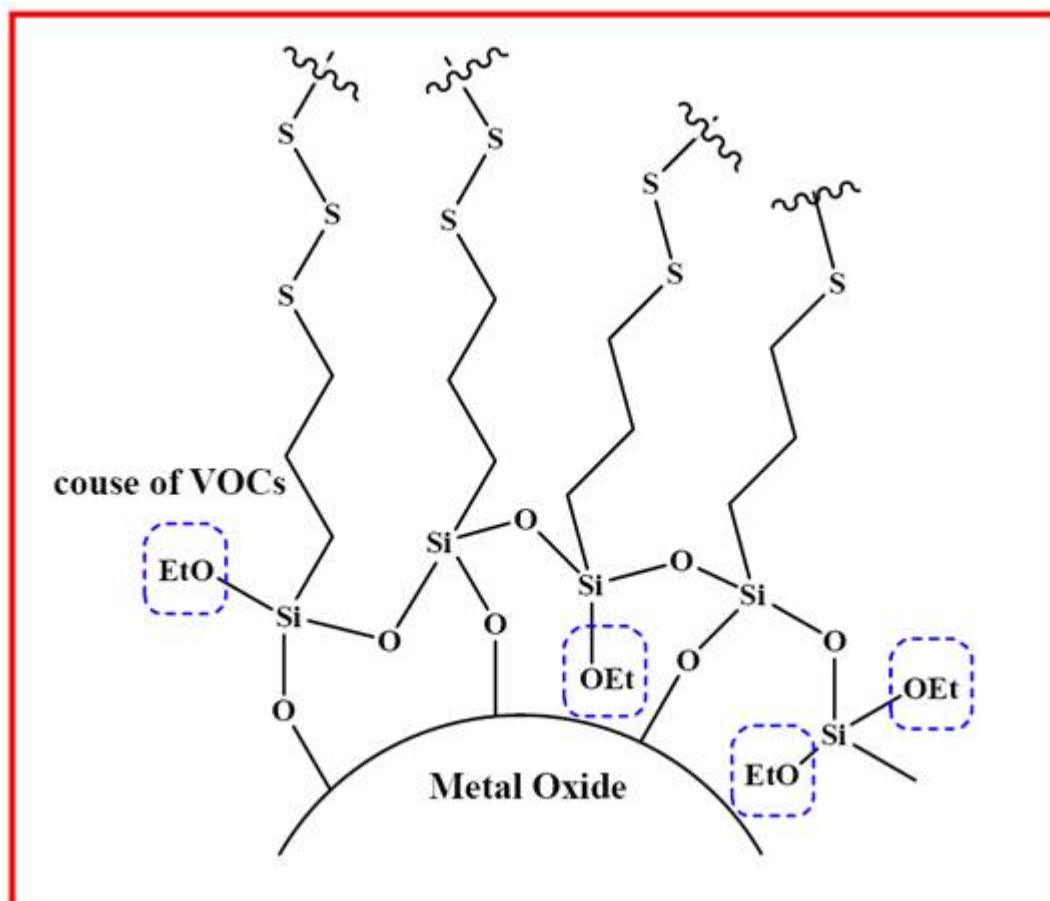
발표종류: 포스터, 발표일시: 목 15:00~17:00

## Reinforcement of SBR Compound with Chemically Modified Silica

정동익, 이광렬, \*한준수, \*유복렬

고려대 화학과 \*KIST 나노재료센터

The use of silica with sulphur-functional organosilanes, such as 3-mercaptopropyltrimethoxysilane (MPTMS) and bis-(triethoxysilylpropyl)tetrasulphide (TESPT), in SBR compound has increased performance. It is known that MPTMS has disadvantage of short vulcanization time. On the other hand, Bifunctional organosilanes, such as TESPT, are very efficient silica-rubber coupling agents. However, it is known that TESPT cannot be completely hydrolyzed in compounding step. Incomplete hydrolyzed alkoxy-functional groups can cause volatile organic compounds (VOC) and decreased performance in SBR compounds. In this study, completely hydrolyzed TESPT and then treated silica affording hydrophobic and reactive modified silica applicable to tire tread compounds.



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## Dehydrochlorinative Si-C Coupling Reaction of Alkenyl Chloride with Trichlorosilane

이동원, \*한준수, \*유복렬, \*\*이명의

연세대 화학과 \*KIST 나노재료센터 \*\*연세대 화학및의화학과

Alkenyl chlorosilanes such as vinylchlorosilane and allylchlorosilane have been widely employed as coupling agents, which when incorporated at modest levels, enhance many of the physical properties of polymer composites, in organic-inorganic hybrid materials industry. As a conventional method, synthesizing alkenylchlorosilanes can be prepared by reaction of metallic silicon with alkenylchloride, HCl in the presence of catalyst or reactions of a hydrosilylation with acetylene or butadiene derivatives of the presence of transition metal (specially expensive Pt, Pd). We have studied synthesis of alkenylchlorosilane by simple thermal dehydrochlorinative Si-C coupling reaction of hydrosilane with alkenyl chloride at temperature 400 to 650 °C with out a catalyst. The yields of akenylchlorosilane depend on the reaction temperature, feeding rate, mixing ratio of reactants and reactor type. In this presentation, we will talk about these synthetic reaction and results in detail.

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발표종류: 포스터, 발표일시: 목 15:00~17:00

## 포화 NHC 백금 착물을 이용한 페닐아세틸렌과 삼염화실란의 수소 규소화반응

송진우, \*한준수, \*\*황영애, \*유복렬

KIST \*KIST 나노재료센터 \*\*상명대 화학과

백금계 촉매를 이용한 수소규소화 반응은 유기규소화합물을 합성하는 대표적인 방법으로써 촉매에 의해 활성화된 하이드로실란과 올레핀을 반응시켜 다양한 실용적 유기규소화합물 합성이 가능하다. 본 연구에서는 다양한 포화 NHC-백금계의 신 촉매를 합성하였고, NMR, X-ray 자료를 토대로 촉매의 합성여부를 증명하였다. 또한 이를 이용한 삼염화실란과 페닐아세틸렌의 수소규소화 반응을 진행하였고, 기존 상용화된 촉매인 Karstedt's Catalyst 와 신 촉매의 반응성 및 경향성을 비교하여 알아 볼 것이다.



일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: II-IND.P-156

발표분야: 공업화학

발표종류: 포스터, 발표일시: 목 15:00~17:00

## Synthesis and Application of $\alpha,\beta$ -Dichlorosuccinic Acid, N-( $\alpha,\beta$ -Dichlorosuccinic acid)Glucosamine Derivatives

류성렬

대불대 보건학부

$\alpha,\beta$ -(dichloro or monochloro)succinic acids were synthesized through the reaction of maleic anhydride with  $\text{Cl}_2$  or  $\text{HCl(g)}$ , (UV)250 nm ~ 300 nm wavelength in presence of  $\text{CCl}_4$ . For the second reaction of N-(dichloro or monochloro)succinic acid contained glucosamine derivatives(I,II) was accomplished by a modification of the general acylation using excess  $\alpha,\beta$ -(dichloro or monochloro)succinic anhydride in the presence of 2% acetic acid with methanol condition as a solvent at elevated temperature( $70^\circ\text{C}$ ). We considered organic acid derivatives were useful especially for treatment for the cultivating porphyra.

일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: II-INOR.P-157

발표분야: 무기화학

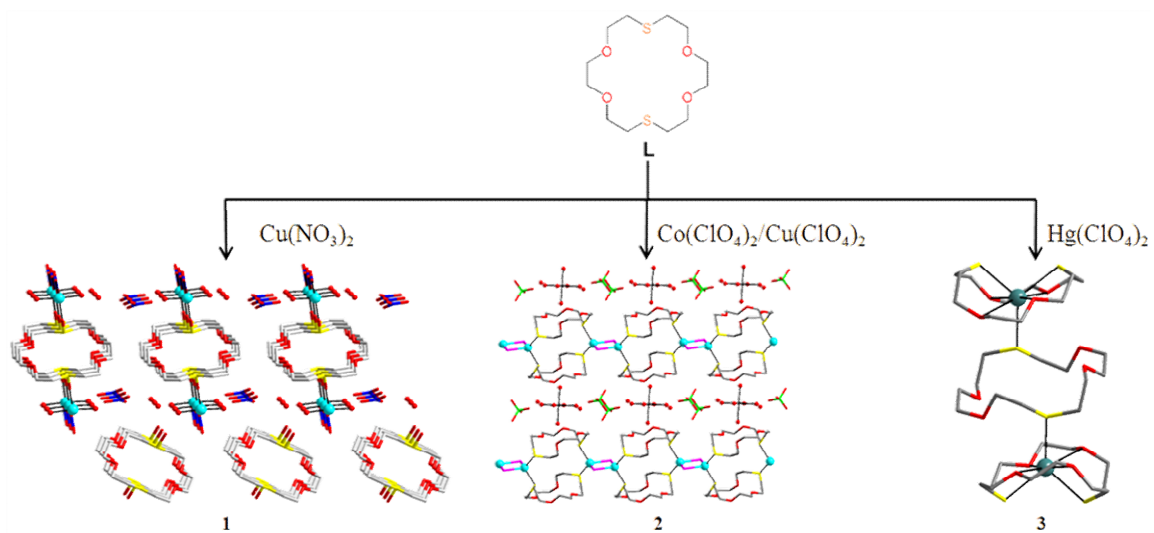
발표종류: 포스터, 발표일시: 목 15:00~17:00

## Preparation and Characterisation of Divalent Hard and Soft Metal Complexes of 1,10-Dithia-18-crown-6: Endocyclic Complexes and Exocyclic Coordination Networks

박인혁, 이심성

경상대 화학과

Since 1,10-dithia-18-crown-6 (L) was synthesized by R. M. Izatt group in 1970, a limited number of crystal structures of its complexes had been reported even though L is expected to have coordination ability for a range of transition metal ions. Thus, we have tried the metallation of L and obtained new 12 complexes of L with hard and soft metal ions in benzonitrile. All crystal structures of the complexes were characterized by single-crystal X-ray crystallography. For example, reaction of L with copper(II) nitrate gave a unique 1D channel-type product (1) via strong  $\text{Cu}^{\text{II}}\text{-O}_{\text{sufoxide}}$  bonds because L was oxidized to the unexpected disulfoxide macrocycle ( $\text{L}_{\text{ox}}$ ) under present complexation condition, meanwhile the parallel reaction with copper(I) iodide with L in the presence of cobalt(II) perchlorate yielded an emissive double-stranded type L complex (2) linked with  $\text{Cu}_2\text{I}_2$  cores. Among the metal complexes of L,  $[\text{Hg}_2(\text{L})_3](\text{ClO}_4)_4$  (3) with 3:2 (L:M) stoichiometry exhibits interesting triple-decker type structure. We will present and discuss the structural characteristics of others metal complexes of L.



일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: II-INOR.P-158

발표분야: 무기화학

발표종류: 포스터, 발표일시: 목 15:00~17:00

## Nanoporous Metal Organic Frameworks Based on Calix[4]arene Derivative

박기민, 류성미, 이심성

경상대 화학과

Metal-Organic framework (MOF) materials have been extensively explored because of their capability for hydrogen storage. Recently, we synthesized a calix[4]arene derivative with four carboxylic acid ( $H_4CTC$  = Calix[4]arene TetraCarboxylic acid).  $H_4CTC$  is a good candidate for the preparation of various three-dimensional nanoporous MOFs because it has four carboxylic pendants. Herein, we report crystal structures and physical properties a new three-dimensional nanoporous MOFs based on  $H_4CTC$ .

일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: II-INOR.P-159

발표분야: 무기화학

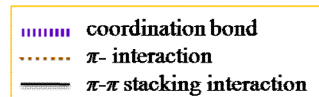
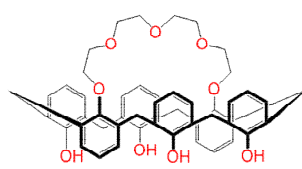
발표종류: 포스터, 발표일시: 목 15:00~17:00

## Molecular Capsules: Homo- and Heterometallic Supramolecular Based on Calixcrown with Multiple Contacts

박인혁, 박기민, \*Jacques Vicens, 이심성

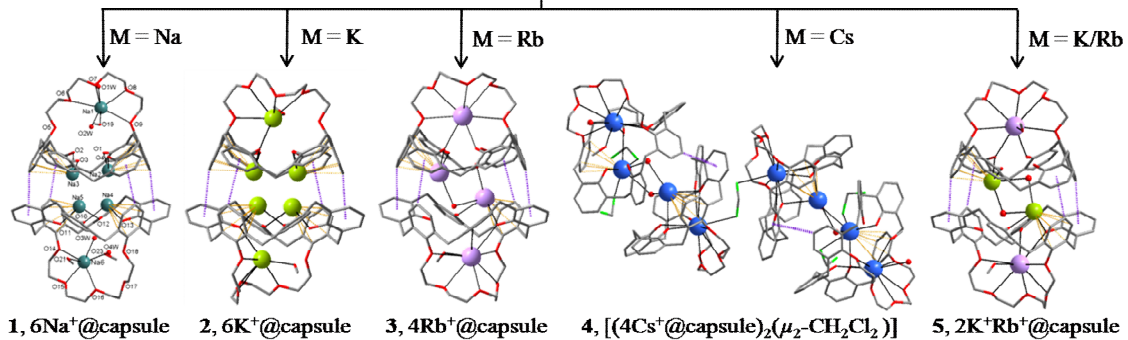
경상대 화학과 \*IPHC-ULP-ECPM-CNRS URA 7178

Assembly of multinuclear alkali metal complexes of calix[6]-*mono*-crowns which can be denoted as ' $nM^+@capsule$ ' are reported. In each capsule-type complex, the two facing calix[6]-*mono*-crown units interact pairwise via edge-to-face  $\pi$ - $\pi$  stacking, adopting a '*capsule*' conformation. We also confirmed that the metal ions are stabilized by multiple contacts such as O(ether)-cation bond, O(phenolate)-cation bond, cation- $\pi$  coordination, cation-solvent coordination and  $\pi$ - $\pi$  stacking interaction. Consequently, this approach enabled us to isolate a totally novel molecular capsule system which contains multinuclear alkali metal including Na<sup>+</sup>, K<sup>+</sup>, Rb<sup>+</sup>, Cs<sup>+</sup>, K<sup>+</sup>/Rb<sup>+</sup> and K<sup>+</sup>/Cs<sup>+</sup> because this system allowed efficient metal-induced dimerization of bowl-type calix[6]-crown unit in a head-to-head fashion that acts as a glue to stabilize this elegant capsule. To the best of our knowledge, these are the first capsule type complexes, in which several homo- and heteronuclear metal ions are encapsulated simultaneously.



Calix[6]-mono-crown-5  
( $H_4L^2$ )

MOH



일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: II-INOR.P-160

발표분야: 무기화학

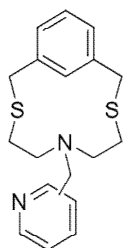
발표종류: 포스터, 발표일시: 목 15:00~17:00

## NS<sub>2</sub>-Donor Macrocycles with Pyridine Arm: Synthesis and Crystal Structures of Ligands and their Supramolecular Complexes

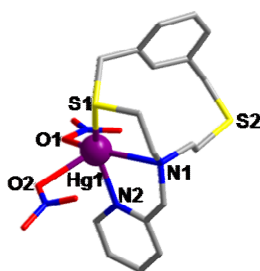
서진우, 박선흥, 이심성

경상대 화학과

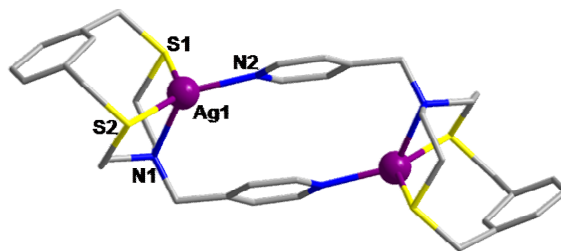
Macrocycles with the pendent arm as an extra binding site have been used not only as new ligands with specific binding properties but also as building block to construct the metallosupramolecules. An isomeric series of monobenzo-N<sub>2</sub>S<sub>2</sub>-macrocycles with a pyridyl arm (*o*-L, *m*-L and *p*-L) were synthesized *via* six steps. Some metal complexes of these ligands were prepared and structurally characterized by X-ray analysis. Reaction of *o*-L with HgCl<sub>2</sub> and Hg(NO<sub>3</sub>)<sub>2</sub> gave an isostructural mononuclear 1:1 (metal-to-ligand) complexes [Hg(*o*-L)X<sub>2</sub>] (1: X = NO<sub>3</sub>, 2: X = Cl), adopting a distorted trigonal bipyramid geometry. However, treatment of *p*-L with Ag(ClO<sub>4</sub>)<sub>4</sub> in same condition afforded a unique cyclic dimer complex [Ag<sub>2</sub>(*p*-L)<sub>2</sub>](ClO<sub>4</sub>)<sub>2</sub> (3). In this case, each silver(I) is in a distorted tetrahedral geometry coordinated by an NS<sub>2</sub> donor set of *p*-L and one pyridine nitrogen from an adjacent ligand photoluminescence study for the ligands and their complexes were also accomplished.



ortho: *o*-L  
meta: *m*-L  
para: *p*-L



1, [Hg(*o*-L)(NO<sub>3</sub>)<sub>2</sub>]



3, [Ag<sub>2</sub>(*p*-L)<sub>2</sub>](ClO<sub>4</sub>)<sub>2</sub>

일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: II-INOR.P-161

발표분야: 무기화학

발표종류: 포스터, 발표일시: 목 15:00~17:00

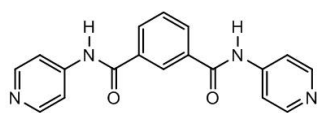
## Metal-Organic Frameworks based on bipyridine and carboxylic ligands with transition metal ions

이은지, 박기민, 이심성

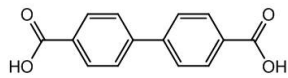
경상대 화학과

Metal-organic frameworks (1-4) with high dimensionality were prepared in the solvothermal reactions of transition metal ions with binary ligand system: bipyridine derivative (L) as an angular ligand and carboxyl ligands ( $H_2BPDC$ ,  $H_3BTC$  and  $H_2BDC$ ). Among the coordination polymers prepared, interestingly, two cobalt(II) complexes with a 3D structure ( $\{[Co(L)(BPDC)] \cdot 4DMF\}_n$  (1) and  $\{[Co_2(L)_2(BPDC)(NO_3)_2] \cdot 4DMA\}_n$  (2) show different network patterns depending on the solvents used. In addition, reaction of L with  $H_2BTC$  and  $Ni(NO_3)_2 \cdot 6H_2O$  also afforded a 3D polymeric array of formula  $\{[Ni_3(L)_3(BTC)_2] \cdot 6DMA\}_n$  (3). Meanwhile, treatment of L with  $H_2BDC$  and  $Zn(NO_3)_2 \cdot 4H_2O$  gave an interpenetrated 2D array of formula  $\{[Zn(L)(BDC)] \cdot 2DMA\}_n$  (4).

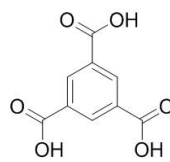




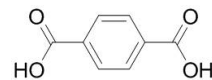
**L**



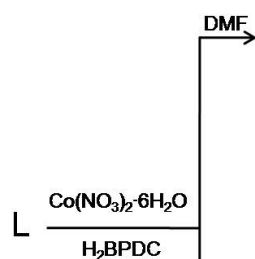
**H<sub>2</sub>BPDC**



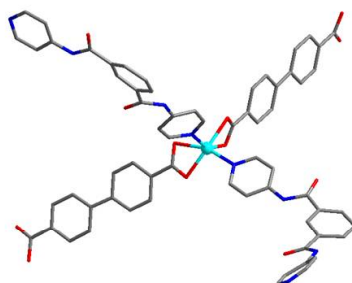
**H<sub>3</sub>BTC**



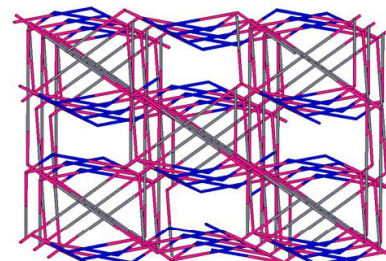
**H<sub>2</sub>BDC**



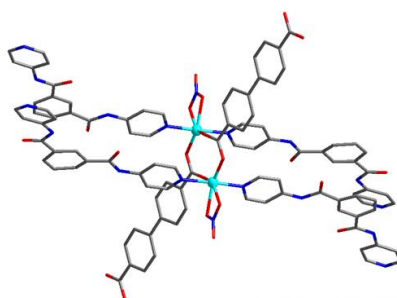
DMF



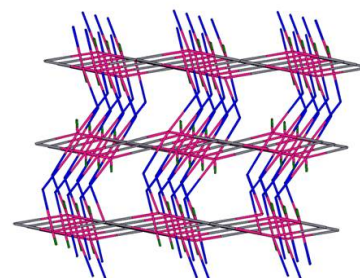
**1, {[Co(L)(BPDC)]·4DMF}<sub>n</sub>**



DMA



**2, {[Co<sub>2</sub>(L)<sub>2</sub>(BPDC)(NO<sub>3</sub>)<sub>2</sub>]·4DMA}<sub>n</sub>**



일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: II-INOR.P-162

발표분야: 무기화학

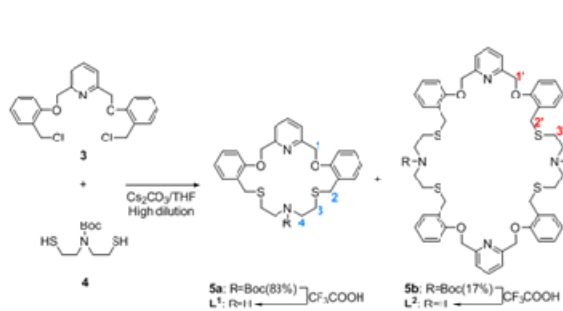
발표종류: 포스터, 발표일시: 목 15:00~17:00

## An Extra Large (XL) Macrocycle: 40-Membered Macrocycle via 2:2 Cyclization and Its Infinite Dimercury(II) Complex

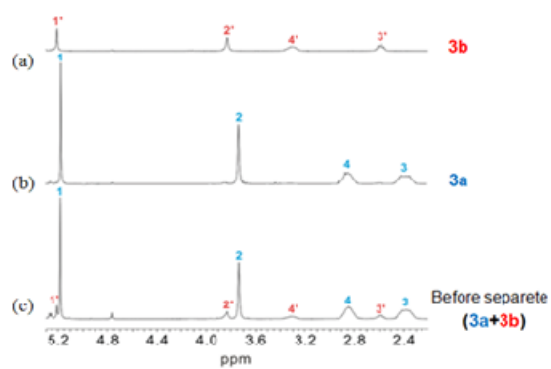
정다람, \*Rie Chamura, \*Yoichi Habata, 이심성

경상대 화학과 \*Department of Chemistry, Toho University, Chiba 274-8510, Japan

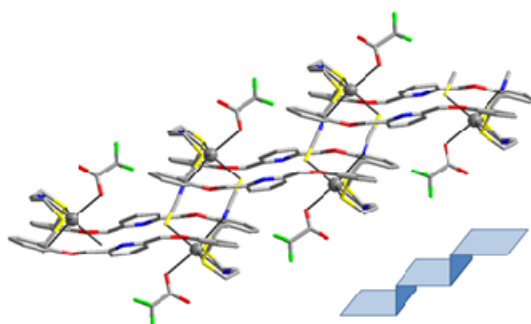
The cyclization of dichloride precursor 1 with N-Boc dithiol 2 led to both N<sub>2</sub>O<sub>2</sub>S<sub>2</sub> (L<sup>1</sup>, 83%) and N<sub>4</sub>O<sub>4</sub>S<sub>4</sub> (L<sup>2</sup>, 17%) macrocycles via 1:1 and 2:2 cyclizations, respectively (See below). We were able to separate the extra larger 2:2 macrocyclic precursor 3b with 40-membered ring size after the optimize the reaction condition. The <sup>1</sup>H NMR spectra of 3a and 3b clearly show the success of the two components from the mixture. The extra large 40-membered N<sub>4</sub>O<sub>4</sub>S<sub>4</sub> macrocycle has allowed to prepare and isolate its dimercury(II) complex [Hg<sub>2</sub>(L<sup>2</sup>)(SCN)<sub>2</sub>(CF<sub>3</sub>CO<sub>2</sub>)<sub>2</sub>]<sub>n</sub>, adopting the 1D stairway-like polymeric chain by further bridging coordination of the anion. The discrete monomercury(II) complex of the smaller 20-membered macrocycle a 1:1 cyclization analog has been also isolated and characterized.



**Scheme 1.** 1:1 and 2:2 cyclizations for  $\text{L}^1$  and  $\text{L}^2$ , respectively



**Figure 1.**  $^1\text{H}$  NMR spectra (aliphatic region) of (a) **3b**, (b) **3a**, and (c) mixture of **3a** and **3b** in  $\text{CDCl}_3$



**Figure 2.** 1D stairway-like polymeric chain



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장소: 제주ICC

발표코드: II-INOR.P-163

발표분야: 무기화학

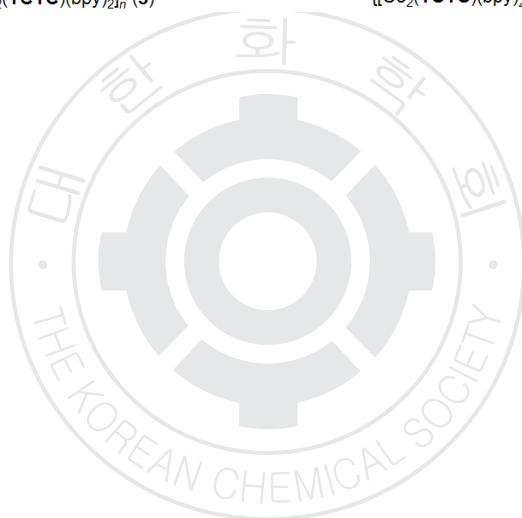
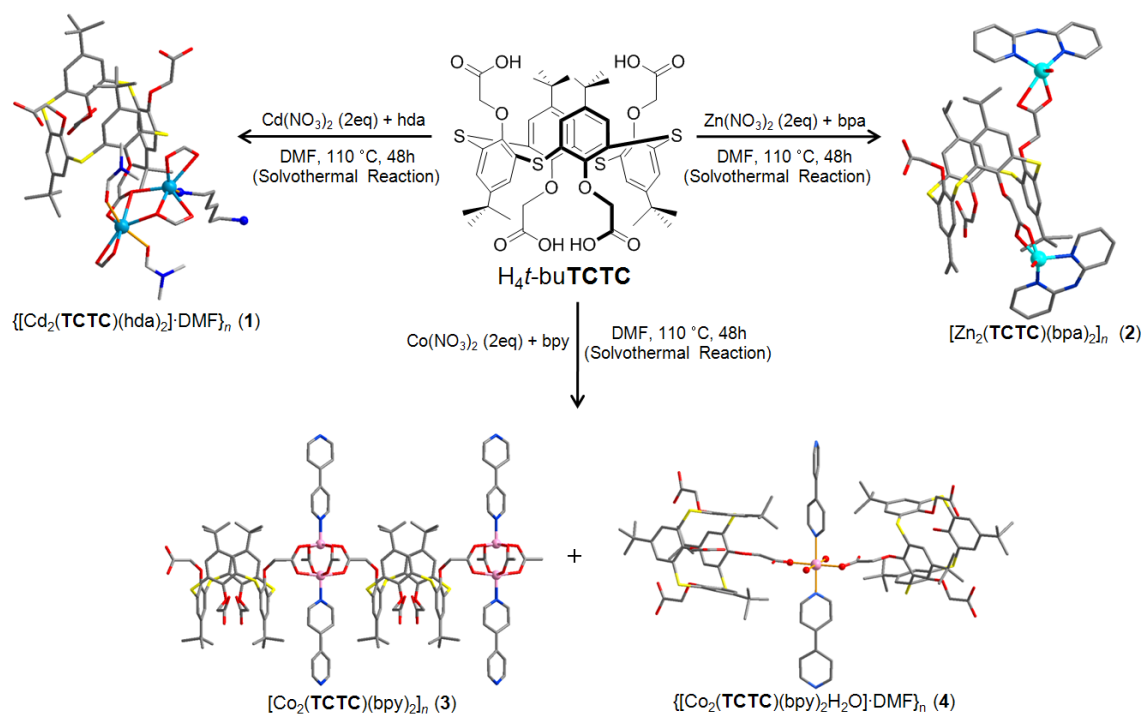
발표종류: 포스터, 발표일시: 목 15:00~17:00

## 3D Metal-Organic Framework incorporating p-tert-Butylthiacalix[4]arene Tetraacetic Acid and Spacer Ligands

김기환, 박선흥, 박기민, 이심성

경상대 화학과

Four supramolecular network complexes (1-4) of p-tert-butylthiacalix[4]arene tetraacetic acid ( $H_4t$ -buTCTC) with cadmium(II), zinc(II), and cobalt(II) in presence of neutral spacer ligands have been synthesized by a solvothermal method and structurally characterized. They are  $\{[Cd_2(TCTC)(hda)_2] \cdot DMF\}_n$  ( $hda$  = diaminohexane) (1),  $[Zn_2(TCTC)(bpa)_2]_n$  ( $bpa$  = 2,2'-bipyridylamine) (2),  $[Co_2(TCTC)(bpy)_2]_n$  ( $bpy$  = 4,4'-bipyridine) (3), and  $\{[Co_2(TCTC)(bpy)_2H_2O] \cdot DMF\}_n$  (4). The extended structures featured with three-dimension (3D) are influenced by the bridging coordination behaviors of the spacer ligands. In these structures, all the  $TCTC^{4-}$  ligands adopt a 1,3-alternate conformation.



일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: II-INOR.P-164

발표분야: 무기화학

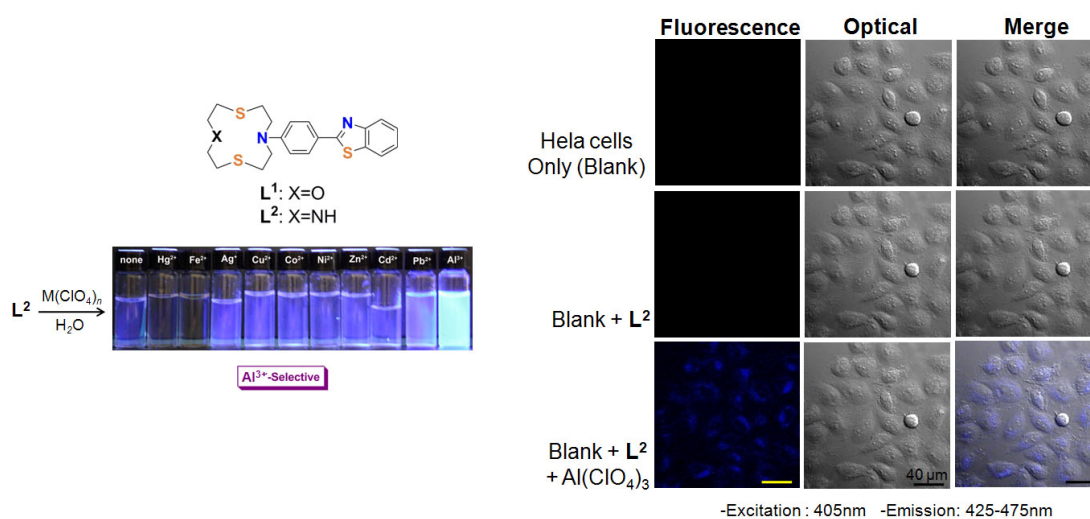
발표종류: 포스터, 발표일시: 목 15:00~17:00

## Benzothiazol-Attached Thiaoxaaza and Thiaaza Macrocycles as A Dual-Photophysical Probe Receptor: Solvent and Anion Effects

박선흥, 이소영, 이심성

경상대 화학과

A benzothiazolyl-group-bearing thiaoxaaza-macrocycle  $L^1$  and thiaaza-macrocycle  $L^2$  were synthesized and their sensing properties for metal ions were investigated through two output channels (color and fluorescence).  $L^1$  showed the selectivity for  $Hg^{2+}$  in terms of hypochromic and fluorescence quenching effects in acetonitrile. In ethanol, however,  $L^1$  exhibited the selectivity for  $Ag^+$ . In case of  $L^2$ , Al(III) showed the largest fluorescence enhancement in water. In ethanol and acetonitrile, however,  $L^2$  exhibited Ag(I)- and Hg(II)-induced fluorescence quenching, respectively. The observed inference of solvent on the metal ion sensing could be explained by the solvation effect on complexation. In addition, the confocal microscopy experiments show that  $L^2$  can be used for detecting  $Al^{3+}$  in Hela cells.



일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: II-INOR.P-165

발표분야: 무기화학

발표종류: 포스터, 발표일시: 목 15:00~17:00

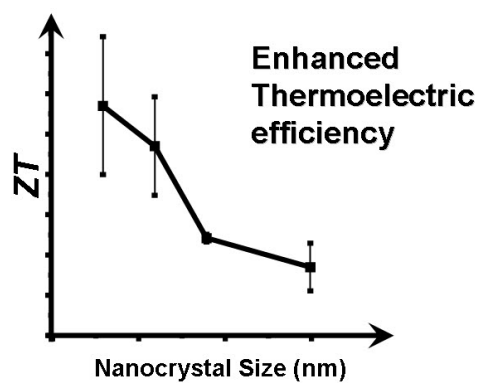
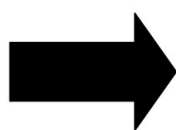
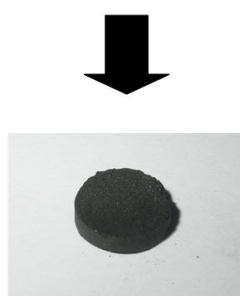
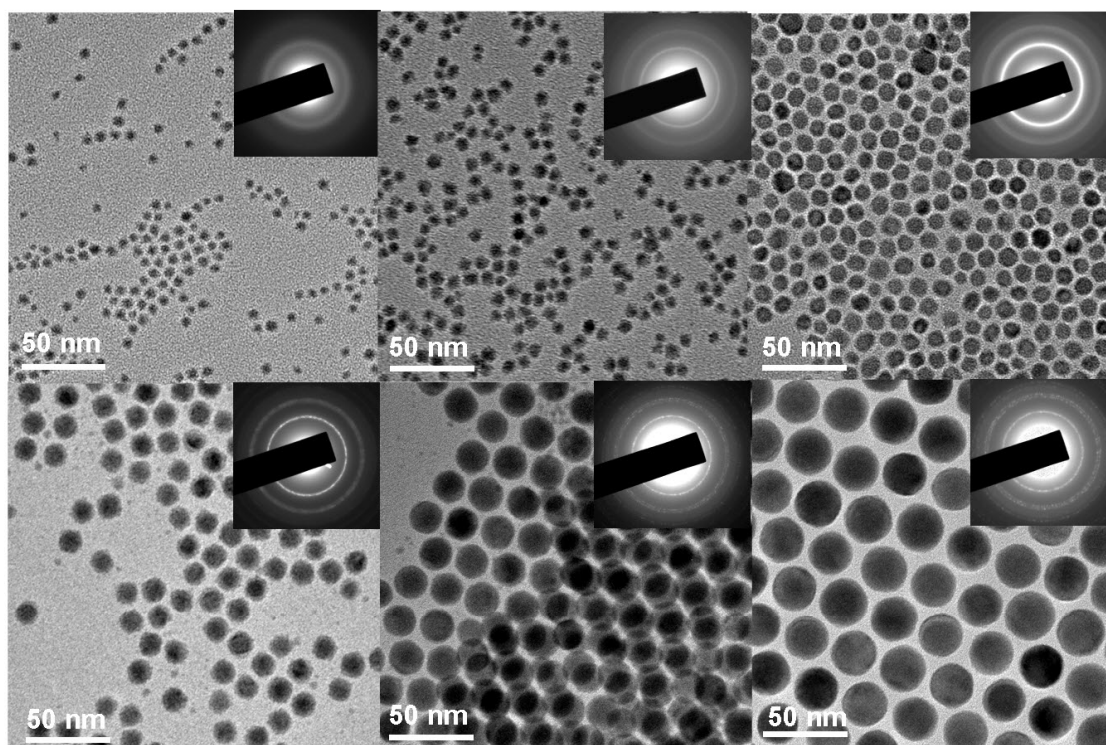
## Large-Scale Synthesis and Characterization of the Size-Dependent Thermoelectric Properties of Uniformly Sized Bismuth Nanocrystals

손재성, 현택환

서울대 나노재료실험실, World Class University (WCU) program of Chemical Convergence for Energy & Environment (C2E2), 화학생물공학부

We here report a very simple and large-scale synthesis of uniform-sized bismuth (Bi) nanocrystals with controlled sizes, and characterized size-dependent thermoelectric properties. Bi nanocrystals were synthesized by the reduction of bismuth thiolate using tri-n-octylphosphine. To characterize the thermoelectric properties, we made pressed nanocrystals by pressing the nanocrystal powder after surfactant exchange with short-chain alkylthiol. The electrical conductivities of the pressed Bi nanocrystals were clearly dependent on nanocrystal size and had significantly high values of  $10^4$ - $10^5$  S/m. Furthermore, the 8 nm sized nanocrystals exhibited extremely low thermal conductivity of  $\sim 0.35$  W/m•K, which is  $\sim 15$ -fold lower than that of bulk Bi and comparable to the insulating limit of solids due to phonon scattering at organic surfactants. Furthermore, size-dependant electrical and thermal properties have been clearly demonstrated using uniform Bi nanocrystals with controlled particle sizes. Interestingly, we found that the ratio of electrical to thermal conductivity increased with decreasing particle size, resulting in the increased ZT value. This enhancement of ZT demonstrates the potential for achieving high ZT values by engineering the size of the nanocrystals. Moreover, the large-scale colloidal chemical synthetic route for uniform-sized nanocrystals offers a way for preparing low-cost thermoelectric materials in large quantities.







일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: II-INOR.P-166

발표분야: 무기화학

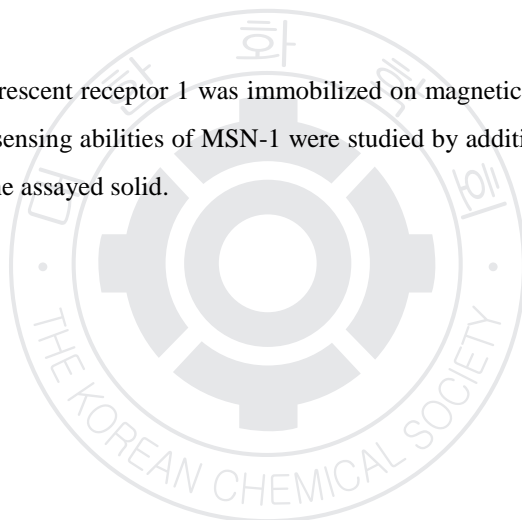
발표종류: 포스터, 발표일시: 목 15:00~17:00

## **Silica-Based Magnetic Nanoparticles for Detection of Fluoride Ion.**

박민성, 정종화

경상대 화학과

Nitrobenzofuran-based fluorescent receptor 1 was immobilized on magnetic silica nanoparticles(MSN-1) via a sol-gel reaction. The sensing abilities of MSN-1 were studied by addition of the anions F<sup>-</sup>, Cl<sup>-</sup>, Br<sup>-</sup>, I<sup>-</sup> to water suspensions of the assayed solid.



일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: II-INOR.P-167

발표분야: 무기화학

발표종류: 포스터, 발표일시: 목 15:00~17:00

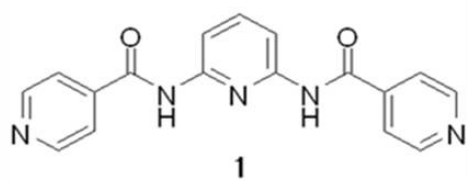
## Pyridine-based Coordination Polymeric Hydrogel with $\text{Cu}^{2+}$ Ion and Its Encapsulation for Hydrophobic Molecule

이혜진, \*이진용, 정종화

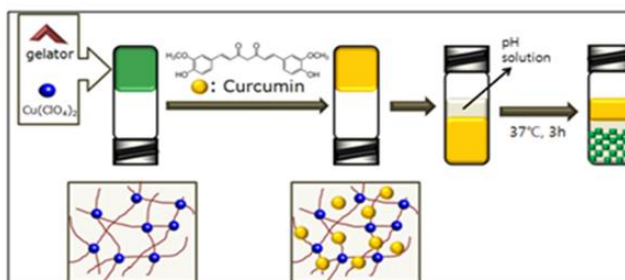
경상대 화학과 \*성균관대 화학과

Compound 1 was synthesized and its gelation ability was evaluated in the absence and the presence of transition metal ions such as  $\text{Cu}^{2+}$ ,  $\text{Co}^{2+}$ ,  $\text{Zn}^{2+}$ ,  $\text{Mn}^{2+}$  in  $\text{MeOH} : \text{H}_2\text{O} = 1 : 1$ . Interestingly, 1 formed gel in the presence of  $\text{Cu}^{2+}$  ion without heating process. Hydrogels possess a range of applications in areas such as tissue engineering, controlled-release drug delivery systems and medical implants. We tested the gel as a delivery vehicle model. We demonstrate pH-triggered delivery at physiological conditions, where we encapsulated a hydrophobic molecule in the coordination polymeric hydrogel and subsequently released the hydrophobic molecule by degrading the gel with weak acid. As a model molecule we chose one of the best-characterized chemopreventive agents, curcumin (or diferuloylmethane), extracted from the root of *Curcuma longa*, which exhibits strong antioxidative, anti-inflammatory and antiseptic properties. 1.0 mL of an aqueous solution ( $\text{pH} = 5$ ) was added to the curcumin encapsulated gel which had been kept at  $37^\circ\text{C}$  for 80 min. Initially, the added solution was colorless. After 80 min, visual changes the gel became broken, and the top solution became yellow in color which indicated that encapsulated curcumin had been released into the solution. This results can be determine by appear peak of 425 nm in UV spectrum. In this poster, we here report the preparation of pyridine-based coordination polymeric hydrogel with  $\text{Cu}^{2+}$  ion and its physical properties such as morphology, fluorescence and drug encapsulation and release properties.

a)



b)



일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: II-INOR.P-168

발표분야: 무기화학

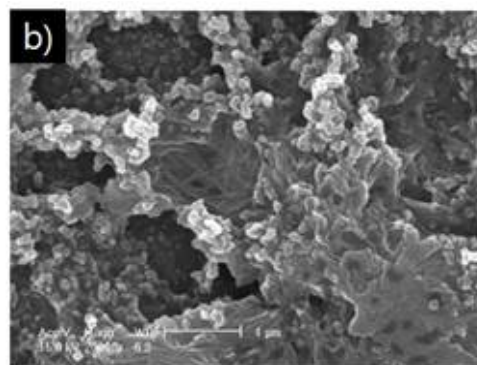
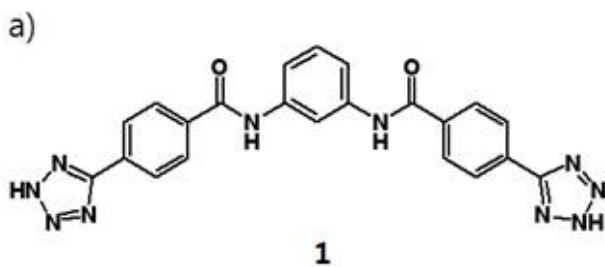
발표종류: 포스터, 발표일시: 목 15:00~17:00

## Tetrazol-based Coordination Polymeric Hydrogel with $Mg^{2+}$

노은영, 이혜진, 정종화

경상대 화학과

Compound 1 was synthesized and its gelation ability was evaluated in the absence and the presence of  $Mg^{2+}$  in water. In addition, the coordination polymeric gel 1 with  $Mg^{2+}$  was evaluated by various anions such as  $NO_3^-$ ,  $SO_4^{2-}$ ,  $I^-$ ,  $Br^-$  and  $Cl^-$ . The coordination gel formation of 1 is independent to anions. The freeze-dried organogel exhibits aggregated spherical or fibrous structures. The fluorescence intensity of the coordination polymeric gel 1 in the presence of  $Mg^{2+}$  is enhanced dramatically with a longer lifetime upon gel formation. In particular, the fluorescence intensity of the coordination polymeric gel 1 was highest in the presence of 2 equivalents of  $Mg^{2+}$  ion. The results indicate that 1 forms the coordination polymeric gel by 1:2 stoichiometry. The coordination polymeric gel may find utility as a novel soft material in biomedical and photochemistry fields.



일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: II-INOR.P-169

발표분야: 무기화학

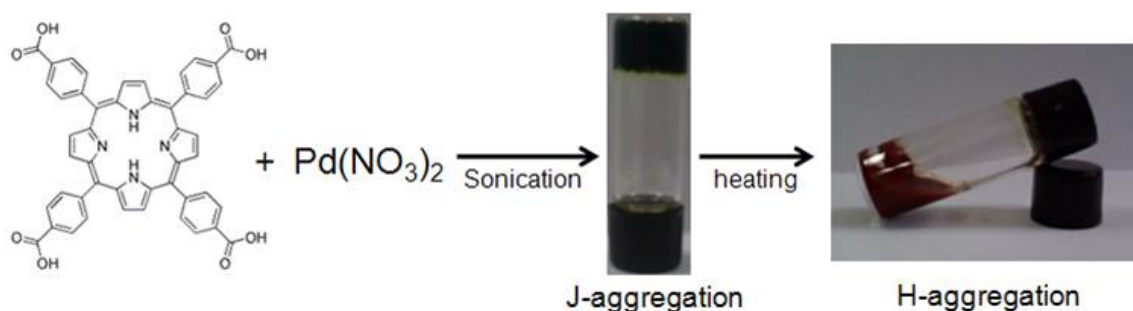
발표종류: 포스터, 발표일시: 목 15:00~17:00

## Remarkable Influence of Porphyrin-Based Metallogel Formation by Ultrasound and Heating: Efficiently Controlled H-and J-types Aggregations

조영제, 정종화

경상대 화학과

The gelation ability of TCPP was tested upon the addition of transition metal ions. Interestingly, TCPP forms the metallogel in the presence of  $\text{Pd}^{2+}$  ion. TCPP- $\text{Pd}^{2+}$  metallogel was characterized by SEM, FR-IR, X-ray diffractometer and Fluorophotometry. When TCPP- $\text{Pd}^{2+}$  metallogel was fabricated in acetonitrile, J-aggregate band were observed at 470 and 668 nm. After heating, the J-aggregates were completely dissociated and an H-aggregate band was observed at 416 nm. The interconversion between the J-aggregates and H-aggregates in the TCPP- $\text{Pd}^{2+}$  metallogel was controllable by heating process. In this conference, we will detail present TCPP metallogel.



일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: II-INOR.P-170

발표분야: 무기화학

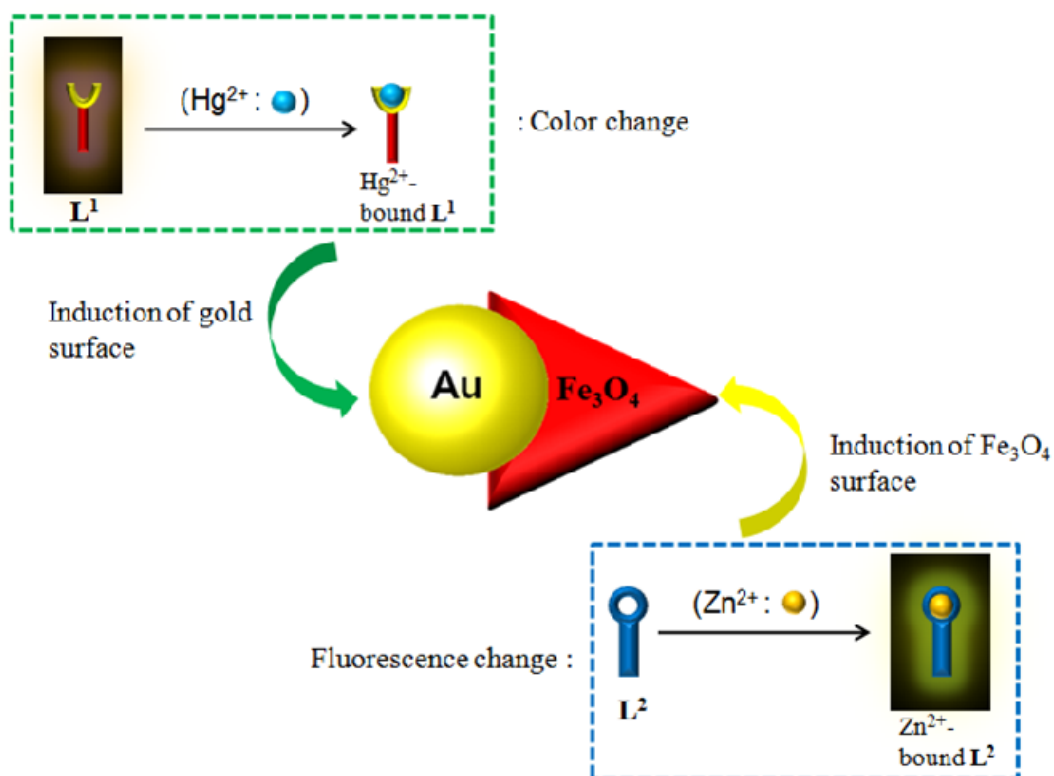
발표종류: 포스터, 발표일시: 목 15:00~17:00

## **Immobilization of Two Different- BODIPY Based Derivative Ligands onto Surfaces of Gold and Fe<sub>3</sub>O<sub>4</sub> Nanoparticles and Its Application as Chemosensor**

손현중, 정종화

경상대 화학과

We synthesized two different chromogenic ligands, which have selectively recognized for Hg<sup>2+</sup> and Zn<sup>2+</sup> ions, respectively. Two different-type ligands were attached onto the gold and Fe<sub>3</sub>O<sub>4</sub> surface of nanoparticles by sol-gel reaction. We observed the chromogenic and fluorogenic changes of Two different ligands immobilized gold and Fe<sub>3</sub>O<sub>4</sub> nanoparticles upon the addition of metal ions in aqueous solution. Two different ligands immobilized gold and Fe<sub>3</sub>O<sub>4</sub> nanoparticles selectively recognized for Hg<sup>2+</sup> and Zn<sup>2+</sup> by each ligands attached onto surface of gold and Fe<sub>3</sub>O<sub>4</sub> nanoparticles.



일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: II-INOR.P-171

발표분야: 무기화학

발표종류: 포스터, 발표일시: 목 15:00~17:00

## Controlled Drug Delivery with Mesoporous Silica as a pH-Response Release System with a Host-Guest Interaction

진달샘, 서무룡, 정종화

경상대 화학과

Phenanthroline-functionalized mesoporous hollow silica nanoparticles (P-MHS) were employed as a typical carrier for host-guest complexation. The controlled release of a model drug molecule in P-MHS was carried by changing pH values. The curcumin selected as a model drug molecule was efficiently encapsulated with the phenanthroline- $\text{Cu}^{2+}$  complex onto P-MHS by coordination bond. The curcumin encapsulated in  $\text{Cu}^{2+}$ -P-MHS was efficiently released into the aqueous phase within 120 min at  $\sim\text{pH } 5$ . Our work provides a method by which the surface of the porous silica can be functionalized in a well-defined manner.





일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: II-INOR.P-172

발표분야: 무기화학

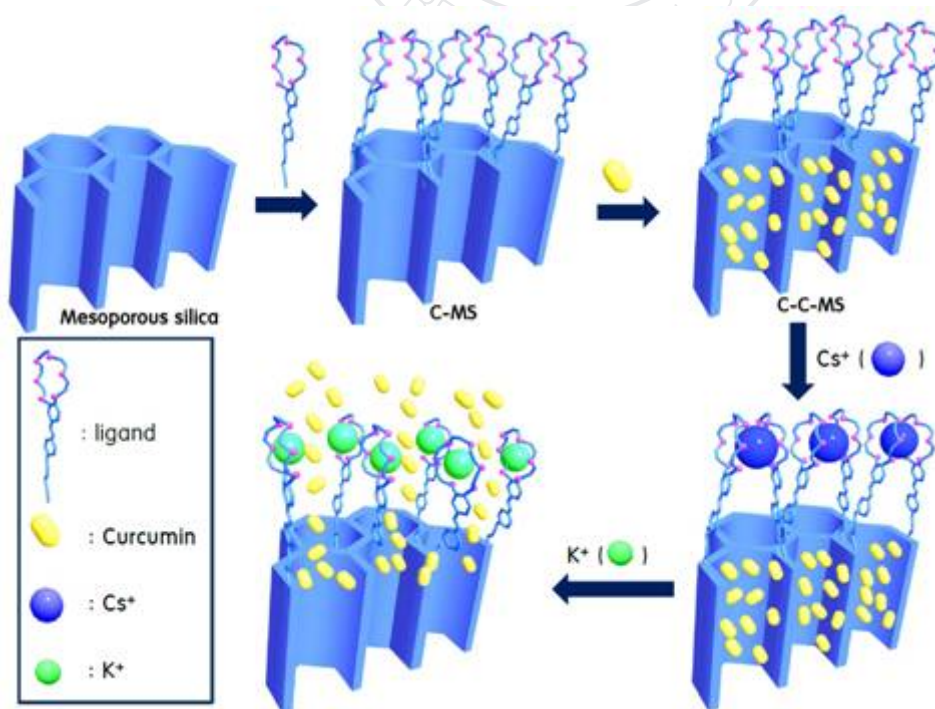
발표종류: 포스터, 발표일시: 목 15:00~17:00

## Controlled delivery using mesoporous silica nanoparticles functionalized with 18-crown-6 derivative

최영란, 정종화

경상대 화학과

Mesoporous silica nanoparticles were functionalized with an 18-crown-6 derivative (C-MS) as a gate molecule. The 18-crown-6 attached to the C-MS formed a complex with a  $\text{Cs}^+$  ion through a coordination bond. When  $\text{K}^+$  ion was added to a  $\text{Cs}^+$ -C-MS encapsulating curcumin, the curcumin was efficiently released into the aqueous phase within 80 min. This work describes a method for functionalizing the surface of a porous silica nanoparticle in a well-defined manner. The C-MS carrier exhibited controlled release of a model drug upon the addition of  $\text{K}^+$  ion.



일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: II-INOR.P-173

발표분야: 무기화학

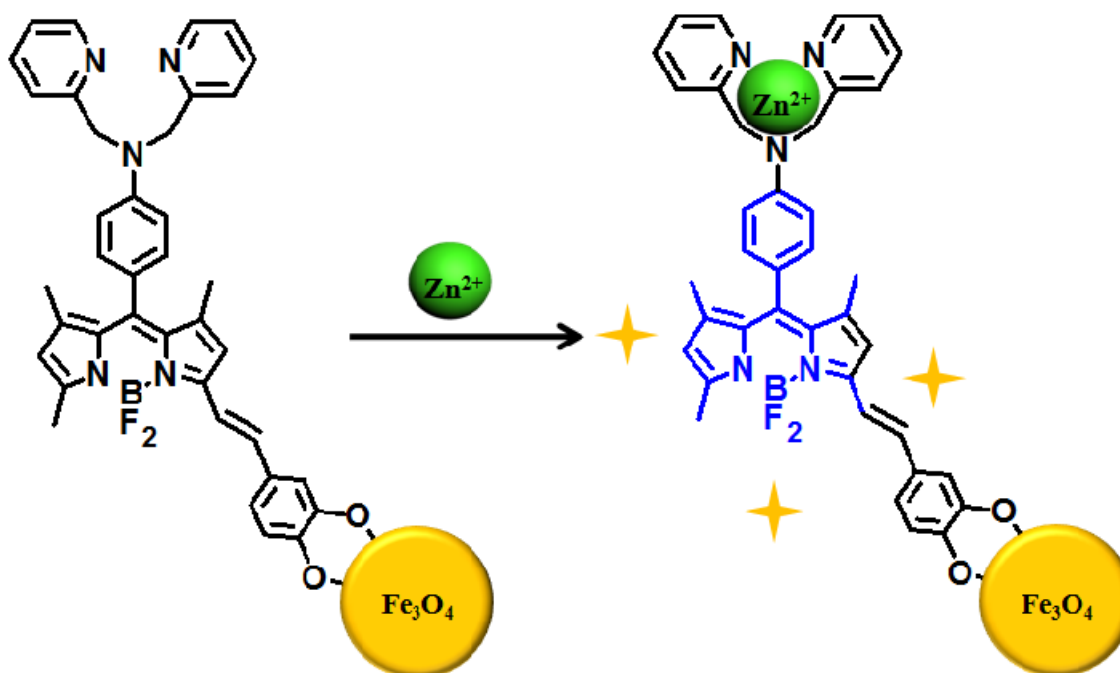
발표종류: 포스터, 발표일시: 목 15:00~17:00

## BODIPY-based fluorescent chemosensor for selective detection of $\text{Zn}^{2+}$ in Aqueous solution

강규식, \*정종화

경상대 나노화학연구실/화학과 \*경상대 화학과

The BODIPY-based ligand was synthesized by several steps and it was immobilized on  $\text{Fe}_3\text{O}_4$  nanoparticles. BODIPY-immobilized  $\text{Fe}_3\text{O}_4$  nanoparticles (1) were characterized by SEM, FT IR, TOF-SIMS, and TGA, and their sensing abilities for metal ions were observed in aqueous solution. The fluorescent intensity of 1 was remarkably enhanced upon the addition of  $\text{Zn}^{2+}$ . On the other hand, no significant changes were observed upon the addition of other metal ions. In this symposium, we will detail present on the fabrication of 1 and its sensing ability for metal ions.



일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: II-INOR.P-174

발표분야: 무기화학

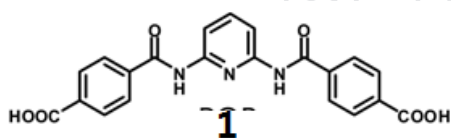
발표종류: 포스터, 발표일시: 목 15:00~17:00

## Graphene-Based Hydrogel

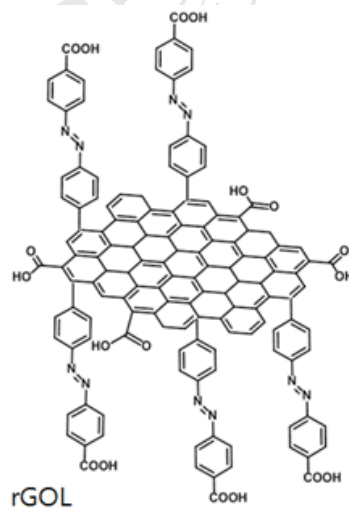
이지하, 서무룡, 정종화

경상대 화학과

The azobenzene-immobilized graphene (A-GO) was prepared by simple organic reaction. A-GO forms the hydrogel in the presence of ligand **1** and  $\text{Zn}^{2+}$ . The hydrogel of A-GO was characterized by SEM, TEM, PXRD, and UV-vis spectroscopy. The hydrogel A-GO showed the rod-like structure.  $T_{\text{gel}}$  of this hydrogel A-GO was  $80^\circ\text{C}$  by observation of DSC. These results indicate that A-GO forms the coordination polymeric structure with  $\text{Zn}^{2+}$ .



0.1M NaOH  
 $\text{Zn}(\text{NO}_3)_2$  3eq



rGOL gel

일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: II-INOR.P-175

발표분야: 무기화학

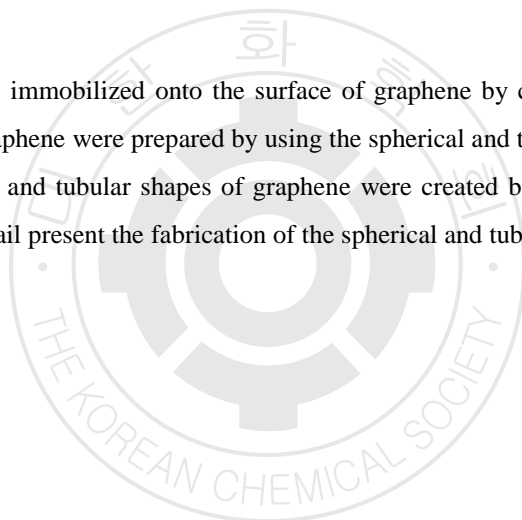
발표종류: 포스터, 발표일시: 목 15:00~17:00

## Shape control of by using inorganic nanomaterials as templates

문승진, 정종화

경상대 화학과

Azobenzene derivative was immobilized onto the surface of graphene by covalent-bond. The spherical and tubular structures of graphene were prepared by using the spherical and the tubular structures of silica as templates. The spherical and tubular shapes of graphene were created by electrostatic interaction. In this conference, we will detail present the fabrication of the spherical and tubular structures of graphene.



일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: II-INOR.P-176

발표분야: 무기화학

발표종류: 포스터, 발표일시: 목 15:00~17:00

## **Transformation of hydrophobic iron oxide nanoparticles to hydrophilic and biocompatible maghemite nanocrystals for highly efficient MRI contrast agent**

박용일, \*박원철, 현택환

서울대 화학생물공학부 \*서울대 융합과학기술대학원 나노융합학과

We report a transformation of hydrophobic iron oxide nanoparticles to hydrophilic and biocompatible maghemite nanocrystals by controlled thermal treatment followed by dextran coating. Salt was used as matrix for preventing aggregation during the thermal treatment at high temperature. Through the thermal treatment and subsequent isolation process, highly crystalline bare maghemite nanocrystals with high magnetization were produced. Subsequent coating with dextran derivatives produced hydrophilic and biocompatible iron oxide nanocrystals. Dextran coated nanocrystals exhibited high relaxivity originated from high magnetization and assembled structure.

일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: II-INOR.P-177

발표분야: 무기화학

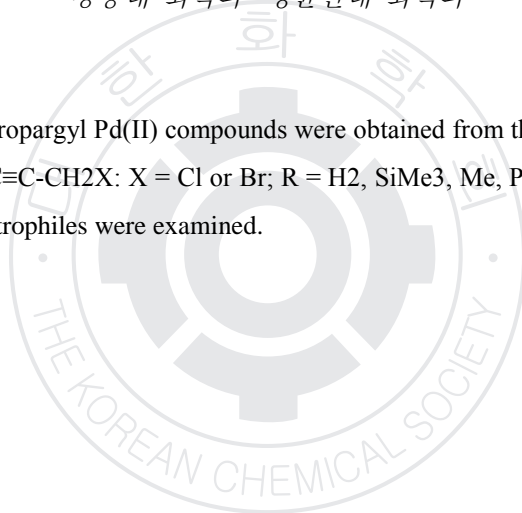
발표종류: 포스터, 발표일시: 목 15:00~17:00

## Synthesis and Properties of New $\sigma$ -Allenyl- and/or Propargyl Pd(II) compounds

김용주, 이정현, 이혁희, 김현경, \*이순원

강릉대 화학과 \*성균관대 화학과

Several  $\sigma$ -Allenyl- and/or Propargyl Pd(II) compounds were obtained from the reactions of Pd(styrene)<sub>2</sub> with propargyl halides ( $R-C\equiv C-CH_2X$ :  $X = Cl$  or  $Br$ ;  $R = H_2, SiMe_3, Me, Ph$ ). Their chemical properties toward nucleophiles or electrophiles were examined.



일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: II-INOR.P-178

발표분야: 무기화학

발표종류: 포스터, 발표일시: 목 15:00~17:00

## **Oxidative Additions of Organic Halides toward Mono or Bis(carbene)Pd(0) complexes**

김용주, 이정현, \*이순원

강릉대 화학과 \*성균관대 화학과

Novel  $\text{PMe}_3\text{-NHC-Pd(0)}$  complexes were obtained from the reactions of  $\text{Pd(styrene)(PMe}_3)_2$  with an equimolar NHC (N-heterocyclic carbene: IPr or SIPr). Additional treatments with NHC ligands to the  $\text{PMe}_3\text{-NHC-Pd(0)}$  complexes produced bis(carbene)Pd(0) compounds. Various oxidative additions of organic halides including dichloromethane and chloroform toward the Pd(0) compounds were examined.

일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: II-INOR.P-179

발표분야: 무기화학

발표종류: 포스터, 발표일시: 목 15:00~17:00

## Synthesis, photoluminescence, and magnetic properties of transition metal complexes with organic ligand including dipyridyl group

신종원, 로투산카라라오, 김승휘, \*조현정, \*민길식

경북대 화학과 \*경북대 사범대학 화학교육과

[Ag(bmp)(NO<sub>3</sub>)]•CH<sub>3</sub>CN•H<sub>2</sub>O (1), [Ag(bmp)(CF<sub>3</sub>CO<sub>2</sub>)] (2), [Cu(bmp)(CH<sub>3</sub>COO)<sub>2</sub>]•2CH<sub>3</sub>OH (3), and [Mn(bmp)<sub>2</sub>(NCS)<sub>2</sub>]•2CH<sub>3</sub>OH (4), have been prepared by the self-assembly of MX or MX<sub>2</sub> (M = Ag, Mn, Cu, X = NO<sub>3</sub><sup>-</sup>, CH<sub>3</sub>COO<sup>-</sup>, and CF<sub>3</sub>COO<sup>-</sup>) with *N*-(pyridin-4-yl)-*N*-(pyridin-4-ylmethyl)pyridin-4-amine (bmp). Complex 1 displays three-dimensional chain-like coordination polymer due to the coordination of nitrate anions with adjacent silver(I) ions, while complex 2 shows two-dimensional framework structure with honeycomb motif along the ac plane. Complex 3 exhibits three-dimensional brick-like coordination polymer due to the geometry of copper(II) ion, while complex 4 shows simple square-like polymer because one pyridine group did not bind to adjacent manganese(II) ion due to the NCS<sup>-</sup> anions. In this poster, we will present the detailed preparation of the bmp ligand and metal complexes, crystal structure, magnetic properties, and luminescent behaviors.



일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: II-INOR.P-180

발표분야: 무기화학

발표종류: 포스터, 발표일시: 목 15:00~17:00

## Synthesis, structure and photoluminescence properties of silver(I) complexes with bis(4-pyridyl)benzylamine

조현정, \*신종원, \*로투산카라라오, \*김승휘, 민길식

경북대 사범대학 화학교육과 \*경북대 화학과

Novel supramolecular solids whose topologies depend on the counteranions,  $[\text{Ag}_2(\text{bpba})_2(\text{NO}_3)_2] \cdot \text{CH}_3\text{CN} \cdot \text{H}_2\text{O}$  (1) and  $[\text{Ag}(\text{bpba})(\text{CF}_3\text{SO}_3)] \cdot 0.5\text{CH}_3\text{CN}$  (2), have been prepared by the self-assembly of  $\text{AgX}$  ( $\text{X} = \text{NO}_3^-$  and  $\text{CF}_3\text{SO}_3^-$ ) with bis(4-pyridyl)benzylamine (bpba). The coordination geometries around silver(I) ions in 1 are a T-shaped and a distorted tetrahedral structures, while silver(I) ion in 2 is a T-shaped structure. Basically, complex 1 displays one-dimensional coordination polymeric structure with 8-shaped along the  $a$ - $b$  axis and also three-dimensional framework structure due to the connection between the 8-shaped chains through nitrate anions. Complex 2 shows one-dimensional zigzag polymer chain along the  $c$ -axis. 1 exhibits a strong visible light emission ranging from violet to red wavelengths, whereas 2 appears a strong visible emission at around 400 nm and a weak visible emission at around 520 nm. In this poster, the detailed preparation of bpba ligand and compounds, crystal structure and photoluminescence properties will be described.

일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: II-INOR.P-181

발표분야: 무기화학

발표종류: 포스터, 발표일시: 목 15:00~17:00

## Template Synthesis of Poly(macrocyclic) Polynuclear Complexes

강신걸, 이윤택, \*정수경

대구대 화학과 \*김포대학 호텔조리학과

A number of polyaza macrocyclic ligands and their complexes have been prepared and investigated. However, examples of polynuclear polymeric complexes containing 14-membered macrocyclic units are quite rare. Various polymeric nickel(II) and/or copper(II) complexes containing 1,3,6,8,10,13-hexaazacyclotetradecane as an integral part of the polymer backbones can be prepared by the reaction of ethylenediamine,  $\alpha,\omega$ -diamines, and formaldehyde in the presence of the corresponding metal ions. Synthesis, characterization, and chemical properties of the poly(macrocyclic) polynuclear complexes are presented.

일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: II-INOR.P-182

발표분야: 무기화학

발표종류: 포스터, 발표일시: 목 15:00~17:00

## Synthesis and Characterization of *C-meso*- and *C-racemic*- Isomers of a Tetraaza Macrocycle Bearing two *N*-cyanomethyl Pendant Arms

강신걸, 방순무, 김현자

대구대 화학과

Two isomers of 1,8-bis(cyanomethyl)-5,5,7,12,12,14-hexamethyl-1,4,8,11-tetraazacyclotetradecane ( $L^2$ ) bearing *N*-cyanomethyl pendant arms, *C-meso*- $L^2$  and *C-racemic*- $L^2$ , have been prepared by the reaction of *C-meso*- $L^1$  or *C-racemic*- $L^1$  ( $L^1$  = 5,5,7,12,12,14-hexamethyl-1,4,8,11-tetraazacyclotetradecane) with bromoacetonitrile. Each isomer reacts with nickel(II) or copper(II) ion to form  $[M(C-meso-L^2)]^{2+}$  or  $[M(C-racemic-L^2)]^{2+}$  ( $M$  = Ni(II) or Cu(II)). Their coordination geometry and chemical properties are influenced by the *C*- conformation of the macrocycle and the nature of the central metal ion. Synthesis and characterization of the macrocycles and their complexes are presented.

일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: II-INOR.P-183

발표분야: 무기화학

발표종류: 포스터, 발표일시: 목 15:00~17:00

## Synthesis of Macrocyclic Nickel(II) and Copper(II) Complexes Bearing Multifunctional Pendant Arms

강신결, 김현자

대구대 화학과

The reaction of acetylacetone, ethylacetoacetate, or diethylmalonate with  $[ML^1]^{2+}$  ( $L^1 = 2,13$ -bis(cyanomethyl)-3,4-dimethyl-2,6,13,17-tetraazatricyclo[16.4.0.<sup>1.18</sup>0<sup>7.12</sup>]docosane) has been examined. The cyanomethyl groups attached to  $[NiL^1]^{2+}$  react with acetylacetone to yield  $[NiL^2]^{2+}$  bearing functional pendant arms containing  $-C(=NH)$  and  $C=O$  groups. The reaction of  $[NiL^1]^{2+}$  with ethylacetoacetate produces  $[NiL^3]^{2+}$  bearing functional pendant arms containing  $-C(=NH)$  and  $COOEt$  groups. The complex  $[NiL^4]^{2+}$  bearing  $-C(=NH)$  and diethylmalonate groups can be prepared by the reaction of  $[NiL^1]^{2+}$  with diethylmalonate in the presence of a base. Synthesis and characterization of the functionalized macrocyclic complexes are presented.

일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: II-INOR.P-184

발표분야: 무기화학

발표종류: 포스터, 발표일시: 목 15:00~17:00

## Synthesis of Macrocyclic Nickel(II) Complexes Bearing Functional Pendant Arms Containing -C(=NH)S- Bonds

강신걸, 김현자, \*곽지훈

대구대 화학과 \*순천대 화학과

The reaction of *N*-cyanomethyl groups of  $[\text{Ni}(\text{L}^1)]^{2+}$   $\text{L}^1 = 1,8\text{-bis}(2,13\text{-bis}(\text{cyanomethyl})\text{-}5,16\text{-dimethyl-}2,6,13,17\text{-tetraazatricyclo}[16.4.0.1^{18}0^{7,12}]\text{docosane})$  with 1-propanethiol or 2-mercaptoethanol produces  $[\text{Ni}(\text{L}^2)]^{2+}$  or  $[\text{Ni}(\text{L}^3)]^{2+}$  bearing functionalized pendant arms containing -C(=NH)-S groups. The reaction is promoted by the central metal ion and is strongly influenced by the nature of the metal ion. Both  $[\text{Ni}(\text{L}^2)]^{2+}$  and  $[\text{Ni}(\text{L}^3)]^{2+}$  readily undergo C-S bond cleavage in basic aqueous solutions. Synthesis and chemical properties of the products are present, along with crystal structure of  $[\text{Ni}(\text{L}^2)]^{2+}$ .

일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: II-INOR.P-185

발표분야: 무기화학

발표종류: 포스터, 발표일시: 목 15:00~17:00

## **New Method for the Improvement of Single Crystal X-ray Diffraction using a High Pressure Cryo-cooling at Pohang Accelerator Laboratory**

문도현

포항가속기연구소 빔라인부

Flash-cooling of single crystals in X-ray diffraction is the best known technique to effectively reduce lost crystallinity in general crystallography. A method of high pressure cryo-cooling is developed and explored at the Cornell High Energy Synchrotron Source (MacCHESS) in USA. The technique involves mounting single crystals from the mother liquor in a cryo-loop with a cryoprotectant oil, pressurizing the crystal to 30,000 psi in helium gas, cooling the crystal under pressure and then releasing the pressure. At the results, dramatic improvement in diffraction quality in terms of resolution and mosaicity was observed in several cases. Recently, this type of equipment has been installed Pohang Accelerator Laboratory (PAL) and modified for small molecule and supramolecule crystallography users. This method can be used to study high pressure effects on metal-organic frameworks (MOFs) and improved to X-ray diffraction for the hollow structures and large cavity structures. We will open this equipment in 2012yr with PLS II upgrade (3.0 GeV 400 mA). The status, equipments and techniques of high pressure cryo-cooling will be presented on this poster.

일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: II-INOR.P-186

발표분야: 무기화학

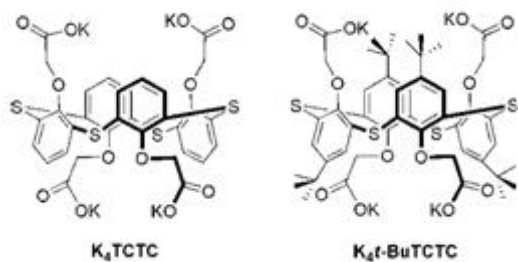
발표종류: 포스터, 발표일시: 목 15:00~17:00

## Thiacalix[4]arene tetraacetate and p-tert-thiacalix[4]arene tetraacetate: their heterobinuclear (K/M: M = Ni, Co, Zn, Ag or Hg) coordination polymers

김기환, 박선흥, 박기민, 이심성

경상대 화학과

Both of potassium salts of thiacalix[4] tetraacetate ( $K_4TCTC$ ) and p-tert-butylthiacalix[4] tetraacetate ( $K_4t-BuTCTC$ ) afforded heterobinuclear (K/M) coordination polymers with the reactions of some transition and other metal ions (M): the former gave an isostructural 1D zigzag networks (when M = nickel, cobalt and zinc),



일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: II-INOR.P-187

발표분야: 무기화학

발표종류: 포스터, 발표일시: 목 15:00~17:00

## Syntheses, Characterization, and Photo-hydrogen-evolving Properties of Bis(bipyridine)(phenanthroline)ruthenium(II) derivatives Tethered to a *trans*-M(II)I<sub>2</sub> (M = Pt, Pd) Unit

박희준, \*김우열, \*최원용, \*\*강윤경, 정영근

서울대 화학부 \*포항공과대 환경공학부 \*\*서울대 화학과

New five complexes of a general formula  $[(N^N)_2Ru(\mu\text{-bridge})_2MI_2]^{4+}$  {  $N^N$  = 2,2'-bipyridine, 1,10-phenanthroline, and 4,4'-di-*tert*-butyl-2,2'-bipyridine; bridge = 1,3-dibutyl-2,3-dihydro-1*H*-imidazo[4,5-*f*][1,10]phenanthroline-2-yl (L1) and 1,3-dimethyl-2,3-dihydro-1*H*-imidazo[4,5-*f*][1,10]phenanthroline-2-yl (L2)} were synthesized, characterized, and their photo-hydrogen-evolving activity (activity to enhance the photochemical reduction of water into molecular hydrogen) was evaluated. In each case, a acetonitrile and water (v/v 1:1) solution containing the  $Ru^{II}_2M^{II}$  (M= Pt, Pd) trimer and TEOA was photolyzed using a 350-W Xe lamp under an Ar atmosphere, during which the amount of H<sub>2</sub> evolved was analyzed by gas chromatography. The best result was obtained in  $[(bpy)_2Ru(\mu\text{-L2})_2PdI_2]^{4+}$ .



일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: II-INOR.P-188

발표분야: 무기화학

발표종류: 포스터, 발표일시: 목 15:00~17:00

## **The bridging ligand based on 1,10-phenanthroline moiety: coordination chemistry and electron transfer studies**

**박희준, \*강윤경, 정영근**

서울대 화학부 \*서울대 화학과

Polynuclear metal complexes have been receiving a lot of attention in many fields of photochemical molecular devices because an electron and/or energy transfer is possible in such complexes. Especially, the bridging ligand connecting each metal site in the supramolecular system is crucial because it determines the extent of electronic communication between each metal unit. Here, a bridging ligand(1,3-dibutyl-2,3-dihydro-1*H*-imidazo[4,5-*f*][1,10]phenanthroline-2-yl) synthesized has two different coordinating sites; diimine and *N*-heterocyclic carbene units. Ru(II)-Rh(I) and Ru(II)-Ir(I) bimetallic complexes containing the bridging ligand have been synthesized and characterized. Furthermore, the electrochemical and photophysical studies showed that an electron transfer of Rh(I) to Ru(II) or Ir(I) to Ru(II) occurred.

일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: II-INOR.P-189

발표분야: 무기화학

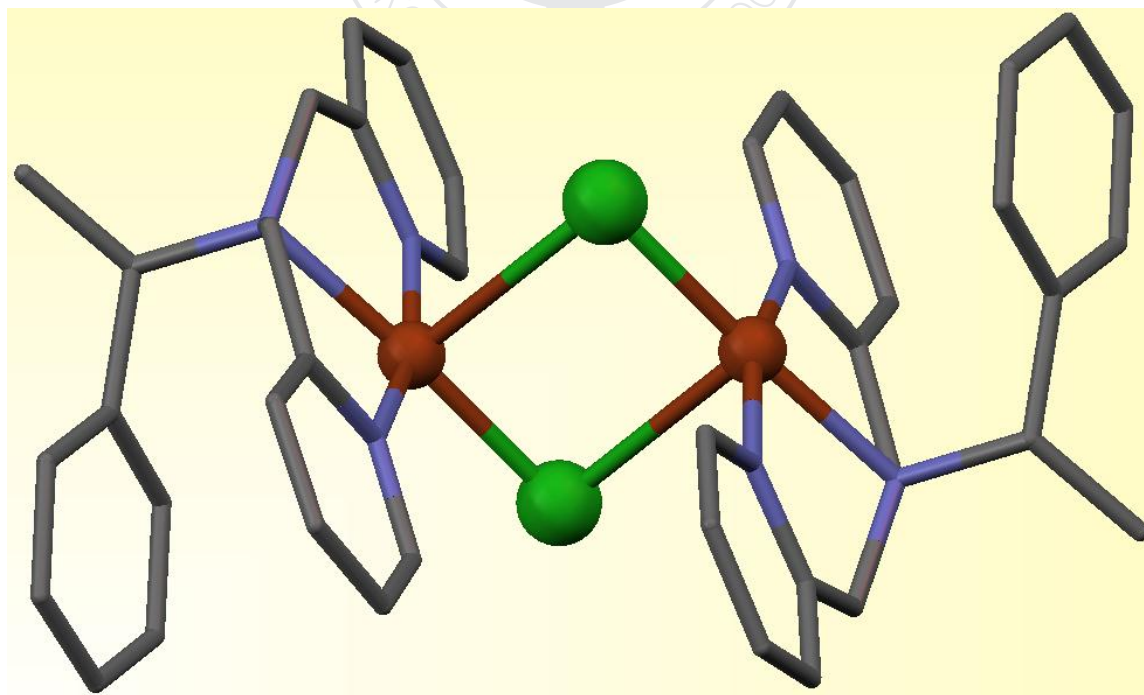
발표종류: 포스터, 발표일시: 목 15:00~17:00

## Dinuclear Cu(II) Complexes with Optically Active and Inactive Tridentate Ligands

김미현, \*김 양, 조정환

고신대 화학신소재학과 \*고신대 화학 신소재학과

We report the synthesis of new optically active and inactive dinuclear Cu(II) complexes of tridentate ligands, 1-phenyl-N,N-bis(pyridin-2-ylmethyl)ethanamine, which were derived from (R)-, (S)- and (RS)-phenylethylamine and picolyl chloride. All complexes were characterized by X-ray crystallography. Each metal ion was linked by two chloride ions as bridge ligand. Spectroscopic and magnetic properties and crystal structures will be reported.



일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: II-INOR.P-190

발표분야: 무기화학

발표종류: 포스터, 발표일시: 목 15:00~17:00

## Synthesis, Structure and Spectroscopic Properties of *cis-β*-[Cr(2,2,3-tet)(N<sub>3</sub>)<sub>2</sub>]Br

최종하, 오세영, \*이상학

안동대 화학과 \*경북대 화학과

The novel complex, *cis-β*-[Cr(2,2,3-tet)(N<sub>3</sub>)<sub>2</sub>]Br (2,2,3-tet=1,4,7,11-tetraazaundecane), was prepared and its structure was determined by single-crystal X-ray diffraction. The complex crystallizes in the space group P2<sub>1</sub>/c of the monoclinic system with a dimensions a=9.1585(7), b=12.2025(10), c=13.8174(11) Å, β = 106.1876(13)° and Z =4. The chromium(III) atom is in a distorted octahedral environment coordinated by four N atoms of 2,2,3-tet and two azido ligands in a mutually *cis-β* geometry. The mean Cr-N(2,2,3-tet) and Cr-N(azide) bonds are 2.084(5) and 2.021(5) Å, respectively. The crystal structure is stabilized by N-H...N(azide) and N-H...Br hydrogen bonds. The IR and electronic spectral properties are also discussed.

일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: II-INOR.P-191

발표분야: 무기화학

발표종류: 포스터, 발표일시: 목 15:00~17:00

## Structure, Spectral and Ligand Field Properties of trans- [Cr(tn)<sub>2</sub>Cl<sub>2</sub>]]ClO<sub>4</sub>

최종하, 오세영, \*유건상

안동대 화학과 \*안동대 응용화학과

The crystal structure of trans-[Cr(tn)<sub>2</sub>Cl<sub>2</sub>]]ClO<sub>4</sub> (tn = 1,3-propanediamine) has been determined by a single-crystal X-ray diffraction study at 185 K. The complex crystallizes in the space group P2<sub>1</sub>/c of the monoclinic system with four mononuclear formula units in a cell of dimensions  $a = 6.4402(4)$ ,  $b = 17.2894(13)$ ,  $c = 13.0851(8)$  Å,  $\beta = 92.899(2)^\circ$  and  $Z = 4$ . The Cr atom is in a slightly distorted octahedral environment coordinated by four nitrogen atoms of two tn ligands and two chlorine atoms in trans position. The orientations of two six-membered rings in the complex cation are in anti chair-chair conformation with respect to each other. The mean Cr-N(tn) and Cr-Cl bond lengths average 2.0862(2) and 2.3112(6) Å, respectively. The ClO<sub>4</sub><sup>-</sup> have slightly distorted tetrahedral geometry with Cl-O lengths and the O-Cl-O angles influenced by hydrogen bonding. The crystal packing is stabilized by several hydrogen bonds. The infrared and electronic absorption spectral properties are also described with the result of X-ray crystallography.

일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: II-INOR.P-192

발표분야: 무기화학

발표종류: 포스터, 발표일시: 목 15:00~17:00

## Synthesis of Silver Nanoparticles from the Deposition of Silver Dicarboxylate Derivatives

이의진, \*PIAO LONGHAI, \*김진권

공주대 에너지시스템공학 \*공주대 화학과

Silver[bis(alkylthio)methylene] malonate was synthesized from the reaction of diethylmalonate and carbon disulfide followed by alkylation, hydrosis and ion exchange. The structure of the Ag complexes were characterized with nuclear magnetic resonance ( NMR ), inductively coupled plasma atomic emission spectrometry ( ICP-AES ) and elemental analysis. Ag nanoparticles ( NP ) was prepared from the decomposition of the Ag complexe using chlorobezene as a reducing agent without an additional stabilizing agent . The size of the Ag NP could be controlled by varying the length of the alkyl chain. The optical properties, crystalline structure and surface composition were characterized by ultraviolet-visible ( UV-vis ) spectroscopy , transmission electron microscopy ( TEM ) , X-ray diffraction ( XRD ) , gas chromatography ( GC-MS ) spectrometry and thermal gravimetric analysis ( TGA ).

일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: II-INOR.P-193

발표분야: 무기화학

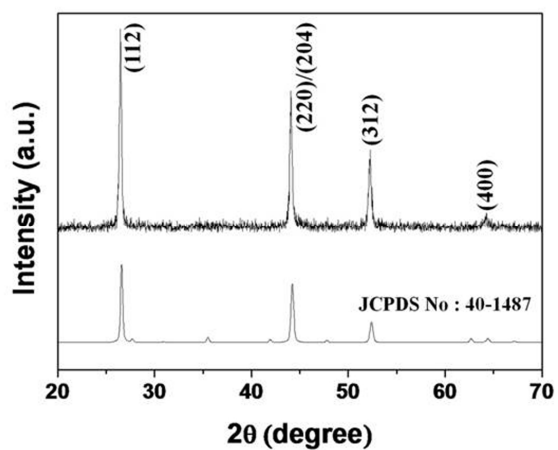
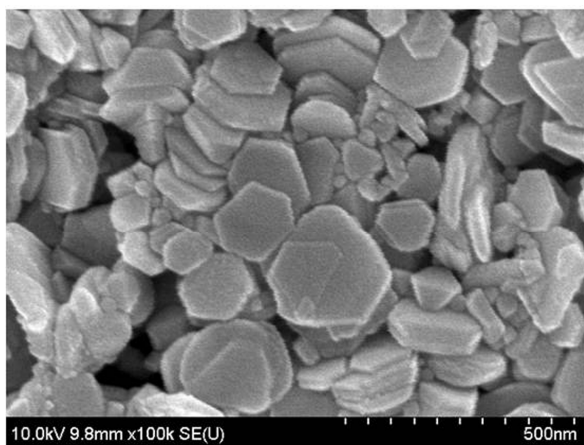
발표종류: 포스터, 발표일시: 목 15:00~17:00

## Synthesis of Tetragonal CuInSe<sub>2</sub> Nanoplates and Their Characterization

Jin Xing, 김진권

공주대 화학과

Copper indium diselenide (CuInSe<sub>2</sub>) is a semiconducting compound which belongs to group I, III and VI chalcopyrite family. CuInSe<sub>2</sub> is a promising material for thin film solar cells because of its extraordinary radiation stability, have band gaps that match well with the solar spectrum, have large absorption coefficients, and avoid the use of overly toxic elements. In past years, solar cells based on CuInSe<sub>2</sub> have been reported with an efficiency of nearly 17%. CISE nanocrystals have previously been made by standard synthetic methods such as solvothermal techniques, Co-evaporation techniques, Electrodeposition and Sputtering techniques. Specially, a solution phase method is not only the cheapest way to make nanocrystals but also helps in making large scale at once. Although several methods have been reported which describe the synthesis of CISE and related Hexagonal plates and tetragonal nanowires, nanoparticles, nanowhiskers, nanorods, nanotubes, nanorings and pyramidal shapes. As a continuation of our previous studies, here, we have synthesized chalcopyrite CuInSe<sub>2</sub> nanoplates using the above sources and coordinating solvent oleylamine followed by complete characterization of the nanoplates. The interesting SEM and XRD images of the synthesized CuInSe<sub>2</sub> nanoplates are displayed below:



일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: II-INOR.P-194

발표분야: 무기화학

발표종류: 포스터, 발표일시: 목 15:00~17:00

## Facile preparation of hollow metal oxide microspheres

박주언, 이희정, 조원, 오문현

연세대 화학과

The hollow micro- and nano-structures have been extensively studied due to their useful properties and applications such as drug-delivery carrier, chemical reactor, and catalyst. The several methods including template-free and templating methods with either hard or soft templates have been developed to fabricate hollow micro- and nano-structures. Herein we report a novel methodology for the preparation of hollow metal oxides. We have demonstrated that considerably monodispersed hollow metal oxides microspheres can be produced from silica@coordination polymer core-shell precursors.



일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: II-INOR.P-195

발표분야: 무기화학

발표종류: 포스터, 발표일시: 목 15:00~17:00

## Self-assembly of $M_{12}L_6$ nanocage

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 선형의 유기 분자와 palladium(II) 착화합물을 자기조립하여  $M_{12}L_6$  타입의 nanocage 화합물을 합성하였다. 관련된 합성과정과 구조 분석 결과를 보고하겠다.

일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: III-INOR.P-1

발표분야: 무기화학

발표종류: 포스터, 발표일시: 금 10:30~12:30

## Effect of Polyacrylate Sodium Modulating the Mineralization of Nano-hematite Crystal

주광건, \*이재범

부산대 나노융합기술대학 \*부산대 나노메디컬공학과

The simulative biomineralization experiments were carried out by hydrothermal synthesis method. Polyacrylate sodium was used as organic matrix in that mineralization system. The purpose was to study the effects of polymer electrolyte on modulating the mineralization behavior of  $\text{Fe}(\text{OH})_3$  gel and its mechanism. The mineralization product were characterization by SEM, XRD, FT-IR method. Moreover, molecular dynamics simulation was used to further investigate the process in order to understand the effect of the polymers on controlling the crystal growth. The results show that polyacrylate sodium could control the crystal structure, morphology, properties by selecting the mechanism of nucleation and transformation. There is the strong complexing action between  $\text{Fe}^{3+}$  iron and the  $-\text{COO}-$  groups of polyacrylate sodium and thus forms a large scale of local supersaturation microenvironment which increased the nucleation driving force of the  $\alpha\text{-Fe}_2\text{O}_3$  crystal. Owing to the existence of the structure matching relation between polyacrylate sodium and  $\alpha\text{-Fe}_2\text{O}_3$  surface, the  $\text{Fe}(\text{OH})_3$  gel transformed the  $\alpha\text{-Fe}_2\text{O}_3$  and inhibited the nucleation of  $\alpha\text{-FeOOH}$ .

일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: III-INOR.P-2

발표분야: 무기화학

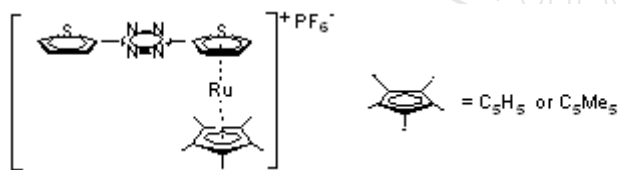
발표종류: 포스터, 발표일시: 금 10:30~12:30

## Synthesis of ( $\pi$ -3,6-bis(2-thienyl)-1,2,4,5-tetrazine)Ru(Cp'=C<sub>5</sub>H<sub>5</sub>, C<sub>5</sub>Me<sub>5</sub>) Complexes

김윤희, 유은정, \*최문근

연세대 화학과 \*연세대 이과대학 화학과

The tetrazine are highly colored and electroactive heterocycles which have a very high electron affinity and low lying  $\pi^*$  orbital, resulting in a  $n\text{-}\pi^*$  transition in the visible light range. These properties make tetrazine based molecules and materials attractive targets for devices targeted for optical and electrochemical applications. In addition, low band gap could be expected from structures alternating tetrazine rings and any electron-rich moiety like thiophene. We will report thiophene substituted tetrazine and preparation of its ruthenium complexes for studies of their electrochemical and photochemical properties.



일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: III-INOR.P-3

발표분야: 무기화학

발표종류: 포스터, 발표일시: 금 10:30~12:30

## Photophysical and Structural Properties of CuI Coordination Polymers with N, S Donor Ligands

김현지, 김태호, 김진은

경상대 화학과

In recent years, copper(I) chemistry has attracted increasing attention because of the 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 two N,S donor ligand, 2-(Cyclohexylthio)-N-(pyridin-4-yl)acetamide, ( $\text{L}^1$ ) and 2-(cyclohexylthio)-N-(pyridin-4-ylmethyl)acetamide, ( $\text{L}^2$ ). And, two Cu(I) coordination polymers 1 and 2 based on the ligands were prepared. Polymers 1 and 2 are composed of rhomboidal  $\text{Cu}_2\text{I}_2$  nodes, polymer 1 is nonemissive under UV irradiation but polymer 2 emits blue light. The results of our investigation including syntheses, structural characterization, thermal and photoluminescent properties of two new Cu(I) coordination polymers are presented.

일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: III-INOR.P-4

발표분야: 무기화학

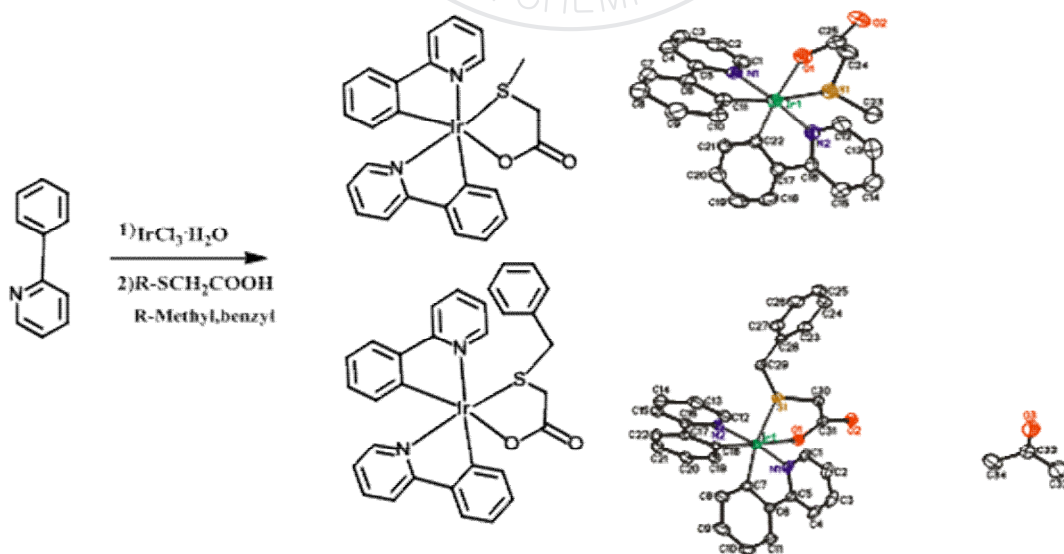
발표종류: 포스터, 발표일시: 금 10:30~12:30

## Phosphorescent Iridium Complexes based on S containing Ancillary Ligand

양호진, 김태호, 김진은

경상대 화학과

Organic light-emitting diodes based on phosphorescent heavy-metal complexes continue to spark a flurry of research activities in scientific community due to the potential application of these compounds as highly efficient electroluminescent emitters. We designed new iridium complexes which contain 2-phenylpyridine as main ligands and new S containing ancillary ligands. Utilizing the synthesized bis-2-phenylpyridine Ir complex and the new two ancillary ligands green-emitting Iridium (III) complexes were synthesized. The results of our investigation including syntheses, structural characterization, thermal and luminescent properties of two new Ir(III) cyclometalated complexes are presented.



일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: III-INOR.P-5

발표분야: 무기화학

발표종류: 포스터, 발표일시: 금 10:30~12:30

## Photoluminescent Properties of Cu(I) Coordination Polymers Based on N/S Donor Ligand

천상훈, 김태호, 김진은

경상대 화학과

Copper(I) halides are capable of adopting a variety of coordination modes ranging from low-dimensional, discrete complexes to 3-D polymeric networks containing various structural motifs,  $(\text{CuI})_x$ , such as rhomboid dimers, cubanes or stair-step tetramers, 1-D chains, and double-stranded stairs, etc. Recently, we have explored coordination polymers based on dithioether ligands and  $(\text{CuI})_x$ . As an extension of our efforts to investigate Cu(I) coordination polymers of dithioether ligands, we introduced an aromatic nitrogen donor instead of a sulfur donor. There are some reports on Cu(I) complexes with N/P mixed donor ligands, N/S mixed donor ligands are still scant. Our investigation focuses on new rhomboid dimer, cubane and stair-step tetramer Cu(I) coordination polymers based on an N/S mixed donor ligand,  $\text{C}_{11}\text{H}_{16}\text{N}_2\text{O}_2\text{S}$ . The results of our investigation including syntheses, structural characterization, thermal and luminescent properties of three new Cu(I) coordination polymers are presented.

일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: III-INOR.P-6

발표분야: 무기화학

발표종류: 포스터, 발표일시: 금 10:30~12:30

## Synthesis and characterization of well-dispersed Nb-doped TiO<sub>2</sub> nanoparticles for solar cell application

김인철, 이원목

세종대 화학과

TiO<sub>2</sub>의 나노 입자 및 얇은 박막필름은 n-형 반도체, 광전소자, 전기변색소자, 광변색소자, 전기발광, 촉매, 화학센서, 태양전지 등 여러분야에 적용되고 있다. 본 실험에서는 기존의 TiO<sub>2</sub>에 Nb가 도핑된 나노입자를 새로운 졸겔법으로 합성하여 높은 성능향상을 추구하였다. 또한 Nb의 도핑 양을 조절 하여 Nb-doped TiO<sub>2</sub>의 결정구조 및 물리적 특성변화가 있는지 알아보았다. 합성한 Nb-doped TiO<sub>2</sub>를 XPS(X-ray photoelectron spectroscopy)으로 나노 입자의 구성성분을 분석하였고 AFM(Atomic Force MicroScope)통하여 Roughness 측정, HR-TEM(High Resolution - Transmission Electron Microscope)을 통한 나노 입자의 형태와 크기분석 그리고 Elipsometry를 사용하여 굴절률 측정 등 다양한 분석을 하여 Nb-doped TiO<sub>2</sub>의 성질을 밝히고자 하였다.

일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: III-INOR.P-7

발표분야: 무기화학

발표종류: 포스터, 발표일시: 금 10:30~12:30

## 포화NHC-Palladium 촉매를 이용한 올레핀과 하이드로실란의 수소 규소화 반응

김현정, 황영애, 강윤경

상명대 화학과

팔라듐계 촉매를 사용하여 하이드로실란과 올레핀을 반응시켜 다양한 유기규소화합물의 합성이 가능하다. 본 연구에서는 새로운 NHC-Palladium 촉매를 합성하였고 NMR 자료를 토대로 촉매의 합성여부를 증명하였다. 또한 이를 이용한 하이드로실란(알콕시실란, 클로로실란)과 탄화수소계 올레핀의 수소규소화 반응을 진행하였고, 기존의 촉매와 신 촉매의 반응성을 비교할 것이다.



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장소: 제주ICC

발표코드: III-INOR.P-8

발표분야: 무기화학

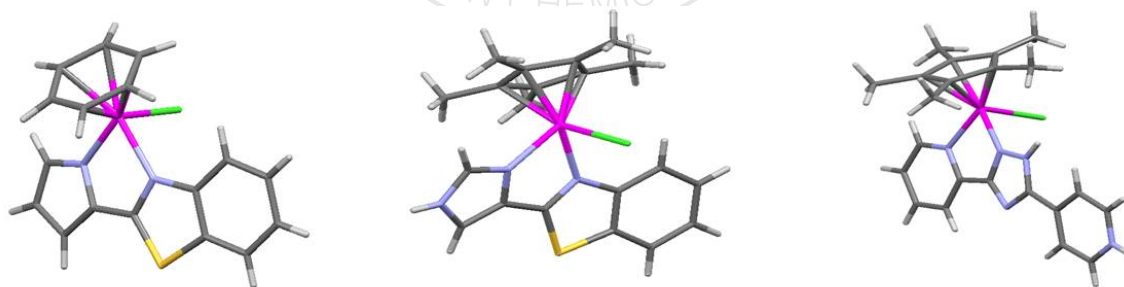
발표종류: 포스터, 발표일시: 금 10:30~12:30

## Antitumor and Cytotoxicity properties of newly synthesized Platinum group metal polypyridyl complexes

GUPTA GAJENDRA, 김진권

공주대 화학과

The DNA binding and cytotoxicity properties of organometallic platinum group metal complexes of the type  $[(\eta^5\text{-Cp}^*)\text{M}(\text{L})\text{Cl}]\text{PF}_6$  where  $\text{M} = \text{Rh}(\text{III})$  and  $\text{Ir}(\text{III})$ ;  $[(\eta^6\text{-arene})\text{Ru}(\text{L})\text{Cl}]\text{PF}_6$  {arene=benzene ; p-cymene and hexamethyl benzene} has been investigated. The antitumor activity was determined in accordance with the US National Cancer Institute (NCI) standard protocol for primary screening in Dalton's lymphoma that was maintained by serial intraperitoneal transplantation. The molecular structures of three complexes were established by single crystal X-ray diffraction studies. They have "piano stool" geometry with  $\eta^5$  and  $\eta^6$  coordination of the arene ligands.



**Figure: Molecular structures of three representative complexes**

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장소: 제주ICC

발표코드: III-INOR.P-9

발표분야: 무기화학

발표종류: 포스터, 발표일시: 금 10:30~12:30

## Synthesis and Characterization of Metal Organic Framework Composed of $\text{MnCl}_2$ and $\text{Ru}(\text{BCN})_2$

공명진, \*정영근

서울대 화학과 \*서울대 화학부

The metal organic frameworks(MOFs) are of great interest due to their potential use in a wide range of applications such as electrochemistry, gas storage, etc.. We especially focused on the electrochemical application of the MOF. Solvothermal reaction of  $\text{MnCl}_2$  and bis[2,6-bis(3-methylimidazol-3-ium-1-yl)pyridine-4-carboxylic acid] ruthenium(II) ( $\text{BCN})_2$  resulted in the formation of 3D-Metalorganic framework. The corresponding geometry was identified as the alternating combination of two different building units by X-ray crystallography. From the solid UV/Vis absorption measurement, light absorption of the MOF turned out to be similar to that of BCN. Energy levels of the HOMO and LUMO were determined by solid cyclic voltammetry.

일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: III-INOR.P-10

발표분야: 무기화학

발표종류: 포스터, 발표일시: 금 10:30~12:30

## Coordination polymers containing 120° bent organic building blocks

설창훈, 조건형, 허정석

충남대 화학과

배위 고분자의 위상구조는 유기 빌딩 블록의 형태와 금속 이온의 배위구조에 따라서 결정된다. 일반적으로 120° 굽은 구조의 유기 빌딩 블록은 paddle wheel 형태의 전이금속 이합체와 조합될 경우 다면체 형태의 중성 착화합물을 형성하는 것으로 알려져 있다. 120° 굽은 구조의 (1,1';3',1'')Terphenyl-4,4''-dicarboxylic acid 화합물과 전이 금속 이온과의 반응에서 얻어진 배위고분자 화합물의 합성과 구조 분석 결과에 대해서 보고하겠다.

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장소: 제주ICC

발표코드: III-INOR.P-11

발표분야: 무기화학

발표종류: 포스터, 발표일시: 금 10:30~12:30

## Anion Effects on Crystal Structures of $\text{Zn}^{\text{II}}$ Complexes Containing 2,2'-bipyridine : Their Photoluminescence and Catalytic Activities

김진훈, 이흥규, \*김 철, \*\*김성진, \*\*\*김영미

서울과학기술대 생무기연구실 \*서울과학기술대 정밀화학과 친환경소재제품센터 \*\*이화여대  
화학과 \*\*\*이화여대 화학-나노과학과

Six new structures of  $\text{Zn}^{\text{II}}$  complexes containing 2,2'-bipyridine (2,2'-bpy) ligands have been determined. For halides, halide anions were used as simple coordinating ligands to form a tetrahedral environment around a  $\text{Zn}^{\text{II}}$  ion. Nitrate and benzoate anions were used as chelating ligands to form an octahedral environment. For non-coordinating  $\text{ClO}_4^-$  and bridging  $\text{SO}_4^{2-}$  anions, three 2,2'-bpy ligands chelate a  $\text{Zn}^{\text{II}}$  to form an octahedral environment, and both  $\text{ClO}_4^-$  and  $\text{SO}_4^{2-}$  anions occupy empty positions between metal cations for charge balances. Polymeric structures of  $\text{Zn}^{\text{II}}$ -2,2'-bpy complexes can be produced by hydrogen bonding.  $[\text{Zn}(2,2'\text{-bpy})(\text{O}_2\text{CC}_6\text{H}_5)_2]$  catalyzed efficiently the transesterification reaction of esters with methanol under the neutral conditions, while the rest of compounds showed very slow conversions. Some of these compounds showed intense emissions at room temperature.

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발표코드: III-INOR.P-12

발표분야: 무기화학

발표종류: 포스터, 발표일시: 금 10:30~12:30

## Novel Cd<sup>II</sup> coordination polymers (1-D, 2-D to 3-D) constructed from *cis*-1,2-cyclohexanedicarboxylic acid and various bipyridyl ligands

이홍균, 김진훈, \*김 철, \*\*김성진, \*\*\*김영미

서울과학기술대 생무기연구실 \*서울과학기술대 정밀화학과 친환경소재제품센터 \*\*이화여대  
화학과 \*\*\*이화여대 화학-나노과학과

Four Cd<sup>II</sup>-(e,a-*cis*-1,2-*chdc*) complexes, [Cd(H<sub>2</sub>O)(μ-1,2-*chdc*)(2,2'-*bpy*)] 1, [Cd(μ-1,2-*chdc*)(μ-*bpe*)]<sub>n</sub> 2, [Cd<sub>2</sub>(μ-1,2-*chdc*)(μ-4,4'-*bpy*)<sub>2</sub>]<sub>n</sub> 3A, and [Cd(H<sub>2</sub>O)(μ-1,2-*chdc*)(μ-4,4'-*bpy*)<sub>2</sub>]<sub>n</sub>•3n(H<sub>2</sub>O) 3B (1,2-*chdc* = 1,2-cyclohexanedicarboxylate), with different assistant ligands (2,2'-bipyridine (2,2'-*bpy*), 1,2-bis(4-pyridyl)ethylene (*bpe*), and 4,4'-bipyridine (4,4'-*bpy*)) have been synthesized and their structures were determined. Depending on the assistant ligands, the structures and dimensionalities of Cd<sup>II</sup>-(e,a-*cis*-1,2-*chdc*) complexes has been varied. Two carboxylates in e,a-*cis*-1,2-*chdc* coordinate to Cd<sup>II</sup> ions with (1111) or (1212) connectivity. Photoluminescence study of the compounds 1 and 2 showed that emission spectrum of compound 1 was observed at 348 nm, while relatively weak luminescence was displayed at 516 nm. The thermal stabilities of these complexes were also examined.

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발표코드: III-INOR.P-13

발표분야: 무기화학

발표종류: 포스터, 발표일시: 금 10:30~12:30

## Robust and Efficient Amide-Based Nonheme Manganese(III) Hydrocarbon Oxidation Catalysts: Substrate and Solvent Effects on Involvement and Partition of Multiple Active Oxidants

이홍규, 김진훈, \*김 철

서울과학기술대 생무기연구실 \*서울과학기술대 정밀화학과 친환경소재제품센터

Mononuclear nonheme manganese(III) complexes,  $[\text{Mn}(\text{bpc})\text{Cl}(\text{H}_2\text{O})]$  (1) and  $[\text{Mn}(\text{Me}_2\text{bpb})\text{Cl}(\text{H}_2\text{O})]\text{CH}_3\text{OH}$  (2), were prepared and characterized. Complex 2 has also been characterized by X-ray crystallography. Magnetic measurements revealed that the complexes are high spin ( $S=5/2$ ) MnIII species with typical magnetic moments of 4.76 and 4.95 B, respectively. These nonheme MnIII complexes efficiently catalyzed olefin epoxidation and alcohol oxidation upon treatment with MCPBA under mild experimental conditions. Olefin epoxidation by these catalysts is proposed to involve the multiple active oxidants  $\text{Mn}^{\text{V}}=\text{O}$ ,  $\text{Mn}^{\text{IV}}=\text{O}$ , and  $\text{Mn}^{\text{III}}-\text{OO}(\text{O})\text{CR}$ . Evidence for this approach was derived from reactivity and Hammett studies, KIE ( $k_{\text{H}}/k_{\text{D}}$ ) values,  $\text{H}_2^{18}\text{O}$ -exchange experiments, and the use of peroxyphenylacetic acid as a mechanistic probe. In addition, it has been observed that the participation of  $\text{Mn}^{\text{V}}=\text{O}$ ,  $\text{Mn}^{\text{IV}}=\text{O}$ , and  $\text{Mn}^{\text{III}}-\text{OOR}$  can be controlled by changing the substrate concentration. Moreover, partitioning between heterolysis and homolysis of the O-O bond of a Mn-acylperoxo intermediate ( $\text{Mn}-\text{OOC}(\text{O})\text{R}$ ) was significantly affected by the nature of solvent, and the O-O bond of the  $\text{Mn}-\text{OOC}(\text{O})\text{R}$  proceeded predominantly by heterolytic cleavage in protic solvent. Therefore, a discrete  $\text{Mn}^{\text{V}}=\text{O}$  intermediate appeared to be the dominant reactive species in protic solvent. Furthermore, we have observed close similarities between these nonheme MnIII complex systems and Mn(saloph) catalysts previously reported, indicating that this simultaneous operation of the three active oxidants might prevail in all the manganese-catalyzed olefin epoxidations, including Mn(salen), Mn(nonheme), and even Mn(porphyrin) complexes.

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발표코드: III-INOR.P-14

발표분야: 무기화학

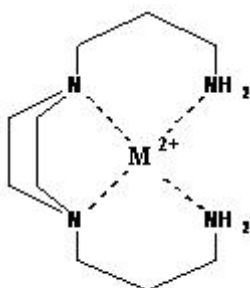
발표종류: 포스터, 발표일시: 금 10:30~12:30

## Synthesis and Structure of Non-cyclic Tetraaza Copper(II) and Nickel(II) Complexes

Enkhzul Otgonbaatar, \*정민철, 곽지훈

순천대 화학과 \*순천대 화학공학과

The complexes of  $[\text{Cu}(\text{L})\text{ClO}_4]\text{ClO}_4$  (1) and  $[\text{Ni}(\text{L})](\text{ClO}_4)_2$  (2) ( $\text{L}$ =1,4-bis(3-aminopropyl) piperazine) have been prepared from the reaction of  $\text{Cu}(\text{ClO}_4)_2 \cdot 6\text{H}_2\text{O}$  or  $\text{NiCl}_2 \cdot 6\text{H}_2\text{O}$  with 1,4-bis(3-aminopropyl) piperazine, respectively, and have been determined crystal structure of them. The structure of 1 consists of  $[\text{Cu}(\text{L})\text{ClO}_4]^+$  cations and  $\text{ClO}_4^-$  counter anions, and perchlorate counter anions. The copper(II) ion of 1 is coordinated four nitrogen atoms of the tetraaza ligand, and an oxygen atom of perchlorate group in a square-pyramidal arrangement and the nickel(II) ion of 2 is four coordinated with four nitrogen atoms of 1,4-bis(3-aminopropyl) piperazine ligand, in a square-planar arrangement. In this presentation, preparation and X-ray structure of 1 and 2 are discussed along with the afforded network structures in crystalline solids.



일시: 2011년 4월 28~29일(목~금) 2일간

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발표코드: III-INOR.P-15

발표분야: 무기화학

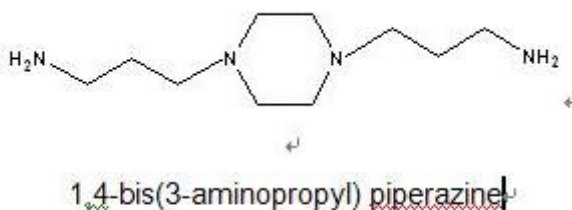
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## Design and preparation of cyano-bridged complexes of copper (II) and nickel(II) complex cooperated by $[\text{Ni}(\text{CN})_4]^{2-}$

Enkhzul Otgonbaatar, 곽지훈

순천대 화학과

Cyano-bridged tetracyanonickelates,  $[\text{Ni}(\text{CN})_4]^{2-}$ , are suitable model compounds for structural and magnetic studies of such systems at low temperatures, because the tetracyanonickelate anion may bridge paramagnetic ions partially coordinated with amine ligands and thus to form molecular, 1D, 2D and 3D structures. The cyano-bridged complexes  $[\text{Cu}(\text{L})]_2[\text{Ni}(\text{CN})_4](\text{ClO}_4)_2$  (1) and  $[\text{Ni}(\text{L})][\text{Ni}(\text{CN})_4]$  (2) ( $\text{L}$ =1,4-bis(3-aminopropyl) piperazine) have been obtained by the reaction of the mixture of  $\text{Cu}(\text{L})(\text{ClO}_4)_2$  and  $\text{K}_2[\text{Ni}(\text{CN})_4]$  in water. The  $[\text{M}(\text{L})]^{2+}$  and  $[\text{Ni}(\text{CN})_4]^{2-}$  fragments linked by two cyanide ligands of the bridged  $[\text{Ni}(\text{CN})_4]^{2-}$  anion and giving  $\text{M}-(\text{NC})-\text{Ni}-(\text{CN})-\text{M}$  linkage. In this presentation, the preparation and X-ray structure of obtained complexes will be discussed in detail.





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발표코드: III-INOR.P-16

발표분야: 무기화학

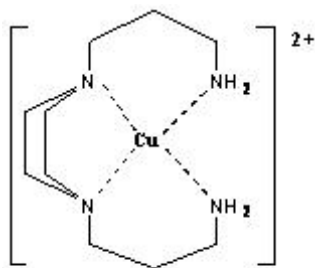
발표종류: 포스터, 발표일시: 금 10:30~12:30

## Preparation and Crystal Structure of Supramolecules from the Combination of Copper(II) Complex of 1,4-Bis(3-aminopropyl)-piperazine and $[\text{Fe}(\text{CN})_6]^{3-}$ or $[\text{Fe}(\text{CN})_6]^{4-}$

Enkhzul Otgonbaatar, \*정민철, 곽지훈

순천대 화학과 \*순천대 화학공학과

Hexacyanometallates, ferricyanide and ferrocyanide are cooperated with various cationic complexes in solution giving cyanide-bridged complexes. These hexacyanometallates are suitable as building blocks to combine with coordinatively unsaturated systems to produce multidimensional structures. Cyanide-bridged multimetallic assembled moieties based on hexacyanometallic building blocks,  $[\text{M}(\text{CN})_6]^{n-}$ , exhibit interesting magnetic and photochemical property. We obtained  $\{[\text{CuL}]_2[\text{Fe}(\text{CN})_6]\}_3[\text{Fe}(\text{CN})_6]$ , (1) and  $[\text{Cu}(\text{L})]_2[\text{Fe}(\text{CN})_6] \cdot 5\text{H}_2\text{O}$ , (2) by the reaction of  $[\text{Fe}(\text{CN})_6]^{3-}$  and  $[\text{Fe}(\text{CN})_6]^{4-}$  as anionic building blocks with  $[\text{CuL}]^{2+}$  complex as a cationic tecton (L=1,4-bis(3-aminopropyl)-piperazine). Here we present the synthesis and X-ray structure of the 1 and 2 in detail.



일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: III-INOR.P-17

발표분야: 무기화학

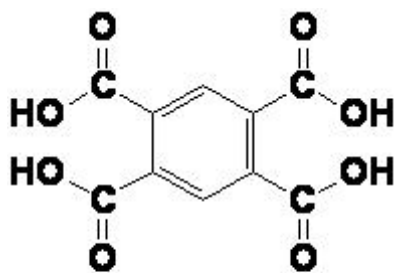
발표종류: 포스터, 발표일시: 금 10:30~12:30

## Molecular Tectonics Using Hexaazamacrocyclic Complexes and 1,2,4,5-Benzenetetracarboxylic Acid (BTCA).

김성민, \*곽지훈

순천대 화학전공 \*순천대 화학과

Crystal engineering is a useful tool to obtain the multidimensional structure by using molecular tectonics. Transition metal complexes containing polycarboxylate ligands have received considerable attention due to their interesting structures and potential applications. Among the various aromatic polycarboxylate ligands, 1,2,4,5-benzenetetracarboxylic acid(BTCA) is especially of interest because of its various coordination features toward the transition metal ions. Here, we present the synthesis, characterization and X-ray structure of the complexes obtained from the combination of hexaaza copper(II) or nickel(II) complexes with 1,2,4,5-benzenetetracarboxylic acid(BTCA) in a various condition such as pH, solvent ect .



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발표코드: III-INOR.P-18

발표분야: 무기화학

발표종류: 포스터, 발표일시: 금 10:30~12:30

## Synthesis and Host Properties of Polynorbornene with 9,9'-(1,3-Phenylene)bis-9H-carbazole (mCP) Side Group in Blue Phosphorescent OLEDs

박준하, 도영규, \*이민형

KAIST 화학과 \*울산대 화학과

Vinyl addition polymerization of norbornene monomer bearing 9,9'-(1,3-phenylene)bis-9H-carbazole (mCP) side group using Pd(II) catalyst has been investigated to produce polynorbornene with pendant mCP groups. The catalytic system efficiently leads to the soluble polynorbornene in combination of 1-octene chain transfer agent. The polymer exhibits high thermal stability with high decomposition and glass transition temperatures. When the polymer was incorporated into the emissive layer as the host doped with various concentration of blue emitter, Flrpic (7-13 wt%) through solution process, all the devices emitted identical blue phosphorescence. The devices displayed the high performances in terms of power efficiency and external quantum efficiency that could be best among the polymeric rivals reported. Details of synthesis, characterization, and host properties of polymer in PhOLEDs will be presented.

일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: III-INOR.P-19

발표분야: 무기화학

발표종류: 포스터, 발표일시: 금 10:30~12:30

## **Molecular Engineering of panchromatic squaraine dye for dye-sensitized solar cells**

백상현, 조나라, 최혜주, 송주만, 유태정, 김철우, 고재중

고려대 소재화학과

Dye-sensitized solar cells (DSSCs) have attracted significant attention due to the low-cost fabrication and high power conversion efficiency. A new series of dye, unsymmetrical panchromatic squaraine sensitizers, which are assembled using both thiophenyl pyrrolyl and indolium groups, exhibit a panchromatic light harvesting up to 780 nm. We already reported panchromatic squaraine sensitizers. However, there were some problems about low open-circuit voltage. So, new sensitizers were designed and synthesised in order to increase Voc as well as electron injection rate through molecular engineering. We expect high efficiency and the device can be applicable to a possible use of "photovoltaic windows" for green house or BIPV.

일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: III-INOR.P-20

발표분야: 무기화학

발표종류: 포스터, 발표일시: 금 10:30~12:30

## Molecular Engineering of Push-Pull Chromophore for Efficient Bulk-Heterojunction Morphology in Solution Processed Small Molecule Organic Photovoltaics

고혜민, 김철우, 백상현, \*이재관, 고재중

고려대 소재화학과 \*호서대 융합기술연구소

The synthesis and characterization of new push-pull chromophores, bisDMFA-diTh-CA, bisDMFA-diTh-MMN, and bisDMFA-diTh-MIMN that are composed of 5'-(4-(bis(9,9-dimethyl-9H-fluoren-2-yl)aniline (bisDMFA) electron donating, dithiophene bridging, and various electron withdrawing moieties, cyanoacrylic acid (CA), methylene malononitrile (MMN), and methylene indenylidene malononitrile (MIMN) were demonstrated for the efficient solution processed BHJ solar cell. The photophysical properties, the hole mobilities from the space charge limitation of current (SCLC) J-V characteristics, and surface morphologies of these materials/PCBM bulk-heterojunction films were also investigated. The best power conversion efficiency of 3.66 % ( $\pm 0.12$ ) with  $J_{sc} = 11.82 \text{ mA/cm}^2$ ,  $FF = 0.35$ , and  $V_{oc} = 0.90 \text{ V}$  was observed in the BHJ film fabricated by bisDMFA-diTh-MMN/C71-PCBM composite with of 3 % 1-chloronaphthalene (CN), which is ~82 % and ~49 % higher efficiencies than before and after post-annealing without treatment of CN, respectively.

일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: III-INOR.P-21

발표분야: 무기화학

발표종류: 포스터, 발표일시: 금 10:30~12:30

## **Small Molecule Bulk Heterojunction Solar Cells based on Dicyanopyran and Tricyanofuran Derivatives As the Donor Materials.**

김주영, 최혜주, 김철우, 도광석, 송주만, 유태정, 고재중

고려대 소재화학과

Organic solar cells are subject to a considerable current interests motivated by the perspective of achieving large area, low-cost, lightweight, and flexible power sources. Solution processable organic semiconductors represent a promising class of new organic photovoltaic (OPV) materials. In this study, Dicyanopyran and Tricyanofuran were introduced into donor-acceptor structure molecule as accepting group in order to lead to an internal charge-transfer band. Dicyanopyran moiety has high thermal stability and Tricyanofuran unit has high molar extinction coefficient and absorbs up to near IR region light. Bulk-heterojunction photovoltaic devices were fabricated using blends of small molecule donor materials and PCBM. The new dyes are appealing candidates in organic photovoltaic.

일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: III-INOR.P-22

발표분야: 무기화학

발표종류: 포스터, 발표일시: 금 10:30~12:30

## **Introducing of fused carbazole unit as electron donor to thiocyanate-free Ru(II) sensitizers for dye sensitized solar cells.**

조나라, 백상현, 유태정, 송주만, 고재중

고려대 소재화학과

Thiocyanate ligands incorporated in most of the ruthenium sensitizers are believed to provide the weakest dative bonding within the metal complexes, making the sensitizers unstable under excessive thermal stress and/or light soaking. This latent inferiority then triggered studies to replace thiocyanate with other effective chelating chromophores in an effort to extend the lifespan of practical solar devices. Herein, we report the preparation of another new class of thiocyanate-free ruthenium sensitizers containing fused carbazole unit as electron donor were synthesized and characterized.

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장소: 제주ICC

발표코드: III-INOR.P-23

발표분야: 무기화학

발표종류: 포스터, 발표일시: 금 10:30~12:30

## Indenothiophene-Functionalized Organic Sensitizers for Efficient Dye-Sensitized Solar Cells

임기민, 송주만, 도광석, \*김점중, 고재중

고려대 소재화학과 \*한국전자통신연구원 차세대태양광연구부

We already synthesized and published ruthenium sensitizers based on Indenothiophene derivative. In this paper, we present new organic sensitizers containing indeno[1,2-*b*]thienothiophene unit. The photovoltaic performance of JK-224 and JK-225 are increased about 20% relatively JK-2. We report here on the synthesis and electrochemical properties of a series of indenothienothiophene-based organic dyes, which have a fluorene derivative as donating group and cyanoacrylic acid as withdrawing group. Consequently we synthesize and develop an efficacious dyes based on indenothienothiophene derivative, and try to discover the reason of high performance through in this study.



일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: III-INOR.P-24

발표분야: 무기화학

발표종류: 포스터, 발표일시: 금 10:30~12:30

## **Study the donor functionalization of chromophores for dye-sensitized solar cells.**

최홍식, 김철우, 최혜주, 고재중

고려대 소재화학과

The demands for alternative power sources have drawn attentions to a variety of light-harvesting devices. Among these, dye sensitized solar cells (DSSCs) have attracted a large number of research groups in two decades. In recent years, many numbers of chromophores with insulating alkyl chains, either on the bridge or the donor units, have been published. It has been shown that the efficiencies and stabilities of the sensitizers are strongly dependent on the position of these insulating alkyl chains. It is well-established that electron-donating groups at the para-position of the triphenylamine phenyls, e.g. alkoxy groups, red-shift the absorption spectrum and increase efficiency, where the degree of red-shift is dependent on the electron-donating strength of the substituent. We have designed and synthesized a sensitizer based on donor group using Fluorene moiety which 5,7-positions are substituted with hexyloxy chains. This dye can be used to study the impact of structural modification on the optical and electrochemical properties.

일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: III-INOR.P-25

발표분야: 무기화학

발표종류: 포스터, 발표일시: 금 10:30~12:30

## Molecular interactions between zinc(II) cyclam and bridging ligands

장충식, \*강민기, \*류충도, 김주창

부경대 화학과 \*부산대학교

New zinc(II) complexes,  $[\text{Zn}(\text{cyclam})(2,6\text{-ndc})]_n$  (1) and  $\{[\text{Zn}(\text{cyclam})(\text{H}_2\text{O})_2](2,6\text{-nds})\}_n$  (2) (2,6-ndc = 2,6-naphthalenedicarboxylate, 2,6-nds = 2,6-naphthalenedisulfonate) have been synthesized and characterized by spectroscopic and crystallographic methods. The complex 1 exhibits 1D polymeric chains with zinc(II) macrocycles and bridging carboxylate ligands. The complex 2 shows a 2D hydrogen-bonded supramolecular structure in which each mononuclear unit is connected by intermolecular hydrogen bonds between the molecules.

일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: III-INOR.P-26

발표분야: 무기화학

발표종류: 포스터, 발표일시: 금 10:30~12:30

## New ruthenium sensitizer based on bipyrrrole ligand for DSSC

김대환, 도광석, 고재중

고려대 소재화학과

Dye-sensitized solar cells (DSSCs) have attracted a lot of interest due to the low-cost fabrication and high power conversion efficiency. In DSSC, ruthenium dyes have shown higher efficiency than organic dye. In this study, new ruthenium sensitizer was synthesized to enhance the stability of metal complex originated from weak bond nature of mono-dentate ligand, isothiocyanate. We introduced bipyrrrole derivative, bidentate ligand, into ruthenium complex instead of isothiocyanate. Herein, we present the synthetic scheme and opto-electrochemical properties of a series of bipyrrrole-based thiocyanate-free ruthenium sensitizers.

일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: III-INOR.P-27

발표분야: 무기화학

발표종류: 포스터, 발표일시: 금 10:30~12:30

## **Synthesis of new acceptor unit, (*E*)-2,3-di(thiophen-2-yl)fumaronitrile, and its application as donor materials for organic solar cells.**

정반석, 김철우, 송주만, 유태정, 도광석, 고재중

고려대 소재화학과

In this study, a new electron acceptor moiety, (*E*)-2,3-di(thiophen-2-yl)fumaronitrile, was synthesized and introduced into the donor-acceptor-donor (D-A-D) structure compounds as core acceptor unit for the application as donor materials of small molecule organic solar cells (SMOPVs). Their optical, electrochemical and thermal properties were examined and bulk-heterojunction (BHJ) photovoltaic devices were fabricated using a blend of the small molecule donor materials and PCBM as an active layer.

일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: III-INOR.P-28

발표분야: 무기화학

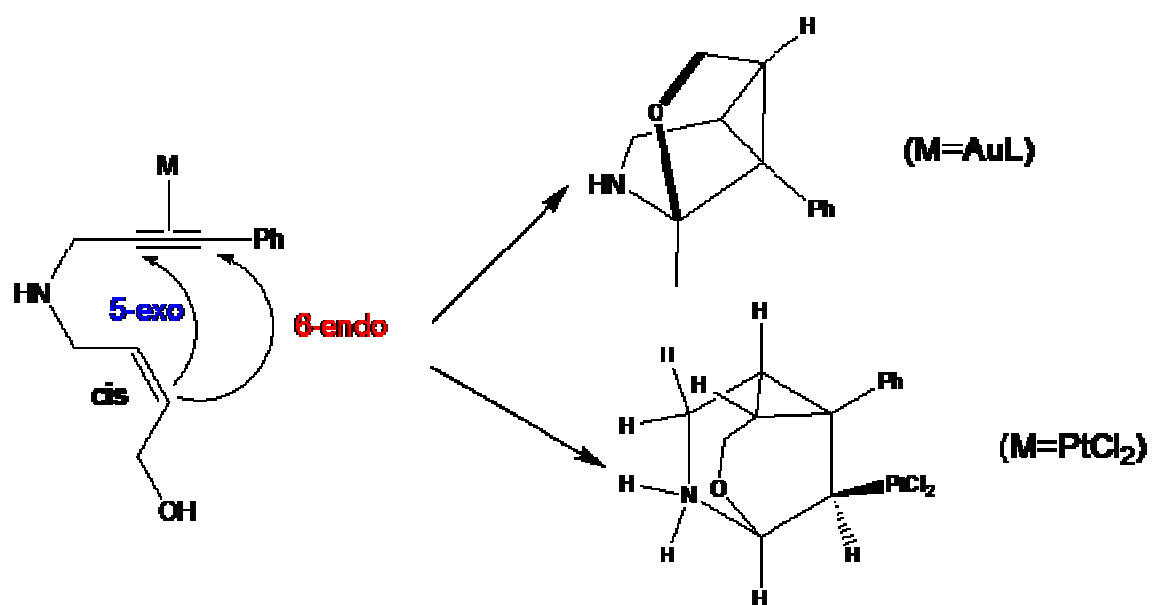
발표종류: 포스터, 발표일시: 금 10:30~12:30

## Computational Study of Gold(I)-and Platinum(II)-Catalyzed Cycloisomerization of Alkynyl Hydroxyallyl Tosylamides

조지은, 강윤경, \*정영근

서울대 화학과 \*서울대 화학부

The transition metal-catalyzed cycloisomerization reactions have attracted much attention due to their synthetic versatility. The selective synthesis of different cyclic products from the same starting materials by simple structural modification or catalyst selection is an interesting but often troublesome topic in such approach. In this regard, Au(I)- and Pt(II)-catalyzed cycloisomerization reactions have been of great interest. Here, we present the theoretical calculation results regarding the reaction mechanism of Au(I)- and Pt(II)-catalyzed cyclization reaction of alkynyl allyl alcohols, which explain the experimental regioselectivity of such catalytic reaction with the different catalyst species. Both reactions are initiated by 6-endo cycloisomerization rather than 5-exo one. But, different kinds of compounds are produced because stabilities of products (called I1 in this research) from this step are different. In Pt(II)-catalyzed reaction case, since I1 is much more stable than reactant R, the stable compound from the directly backside attack. On the other hand, since I1 produced in Au(I)-catalyzed cycloisomerization has similar energy comparing with reactant, we could have found other kinds of reaction channels composed by the interaction of C-N and hydrogen transfer.



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발표코드: III-INOR.P-29

발표분야: 무기화학

발표종류: 포스터, 발표일시: 금 10:30~12:30

## Improved efficiency of over 10% in dye-sensitized solar cells with a ruthenium complex and an organic dye heterogeneously positioning on a single TiO<sub>2</sub> electrode

김철우, 유태정, 송주만, 고재중

고려대 소재화학과

A ruthenium complex (JK-142) with an ancillary bipyridyl ligand substituted by 3-carbazole-2-thiophenyl moiety was synthesized and explored in co-sensitized solar cells in combination with an organic dye (JK-62). The extended  $\pi$ -conjugation in the ancillary ligand makes JK-142 dye have a red-shift light absorption band, while the ineffective penetration of JK-142 molecules to the inner of TiO<sub>2</sub> film due to the big molecular size results in low photovoltaic performance of the single dye sensitized solar cell. Interestingly, when the deficient JK-142 electrode was employed to assemble a co-sensitized solar cell by additionally adsorbing JK-62 dye, a much improved efficiency of up to 10.2% was obtained, which is superior favorably to that (ca. 8.68%) of N719 in the same device configurations. The results shown here not only provide new vision on how to produce high efficient solar cells using dyes with extended molecular structure, but also open up a new way to position different dyes on a single TiO<sub>2</sub> film for co-sensitization through controlling the molecule size.

일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: III-INOR.P-30

발표분야: 무기화학

발표종류: 포스터, 발표일시: 금 10:30~12:30

## **A Ru(III) Complex with a Tripodal Pyrazolyl Tetraamine Ligand :Structure, Spectroscopic Properties, and Peroxidase-like Reactivity**

조장훈, 김동훈, 이흥인

경북대 화학과

Ruthenium complexes have been widely developed to be applied for pharmaceuticals, precursors in a variety of inorganic syntheses, oxo-transfer catalysts, photoinduced energy, water oxidation, and others. Especially, recent advances in pharmaceutical applications of Ru(III) complexes as anticancer drugs have brought much attention to new developments of Ru(III) compounds. Among those, octahedral Ru(III) complexes with chloride and heterocyclic azole ligands have shown promising results. For the clinical success of the complexes, understanding the reactivities of the biomolecule-bound Ru(III) complexes is necessitated. In this study, we have developed a new Ru(III) model complex,  $[\text{Ru(III)(Tpea)Cl}_2](\text{ClO}_4)$ , where Tpea = tris(2-(1-pyrazolyl)ethyl)amine, as a model for the biomolecule-bound Ru(III) complexes. The crystallographic analysis of the complex revealed near perfect octahedral geometry with four N-donor atoms. In-depth study on the catalytic activity of the complex with ABTS [2,2'-azinobis(3-ethylbenzthiazoline-6-sulfonate)] as a co-substrate now reveals the complex has a peroxidase-like reactivity.



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장소: 제주ICC

발표코드: III-INOR.P-31

발표분야: 무기화학

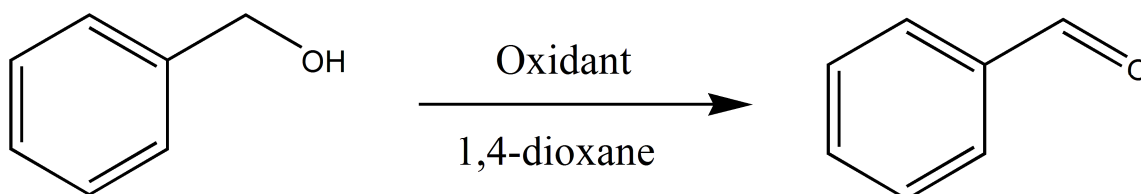
발표종류: 포스터, 발표일시: 금 10:30~12:30

계면활성제를 사용하지 않은 Pd@pSiO<sub>2</sub> 요크-셸 나노구조체를 이  
용한 일차알코올의 선택적산화 (Selective Oxidation of Primary  
Alcohols Catalyzed by The Surfactant-Free Pd@pSiO<sub>2</sub> Yolk-Shell  
Nanostructures)

배희선, \*송현준, 박강현

부산대 화학과 \*KAIST 화학과

The surfactant-free Pd@pSiO<sub>2</sub> yolk-shell structures bearing surfactant-free Pd nanoparticles, prepared through the direct silica coating by the water-in-oil microemulsion method and the pore generation by the partial silica etching and surfactant elimination by the calcinations using high temperature. After the calcinations, the Pd particle size nearly identical to thermally untreated one. This result reflects the high thermal stability of Pd@pSiO<sub>2</sub> yolk-shell structures. This catalyst used for oxidation of primary alcohols to the aldehydes. Aldehydes are useful compounds in the synthesis of fine chemicals such as pharmaceuticals, fragrances or food additives. The selective catalytic oxidation of primary alcohols is one of the most simplest and important approaches to preparation of aldehydes in organic synthesis. The surfactant-free Pd@pSiO<sub>2</sub> yolk-shell catalyst showed a higher catalytic activity in the oxidation of a wide range of primary alcohols and is highly selective to the corresponding aldehydes.



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장소: 제주ICC

발표코드: III-INOR.P-32

발표분야: 무기화학

발표종류: 포스터, 발표일시: 금 10:30~12:30

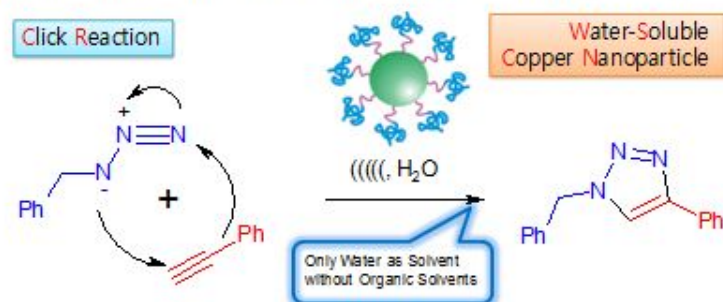
## 이중 친수성 블록 공중합체를 이용한 수용성 구리 나노 입자의 합 성과 클릭 반응에서의 응용 (Double Hydrophilic Block Copolymer Nanoreactor for Synthesis of Copper Nanoparticle and Application in Click Chemistry)

김아람, 박강현

부산대 화학과

Azide-alkyne Huisgen method, which is a Cu(I)-catalyzed cycloaddition between terminal acetylenes and azides at room temperature, is one of the most efficient reactions within the click chemistry philosophy. In this context, we have employed double-hydrophilic block copolymers (DHBCs) in the growth control of inorganic phases such as mineralization with unusual structural specialty and complexity in the aqueous solution. As shown in Table 1, the reaction of benzyl azide and phenylacetylene were studied in the presence of Cu NPs in water. The cycloaddition reaction of benzyl azide and phenylacetylene with water soluble copper nanoparticles in H<sub>2</sub>O, off the shelf, afforded 1,4-disubstituted 1,2,3-triazoles as a single regioisomer. The best results were obtained when H<sub>2</sub>O was used as the solvent, in which sonicated for 10 min with 50% amplitude under 100 °C.

Table 1. Optimization of Click reaction catalysed by Water Soluble Copper NPs.



| Entry | Cat (mol%)        | Temp (°C) | Time (h) | Conv (%) <sup>a</sup> |
|-------|-------------------|-----------|----------|-----------------------|
| 1     | 1 mol% CuO-poly   | 25        | 3        | 3 <sup>b</sup>        |
| 2     | 1 mol% CuO-poly   | 50        | 10 min   | 17                    |
| 3     | 1 mol% CuO-poly   | 100       | 5 min    | 37                    |
| 4     | 1 mol% CuO-poly   | 100       | 10 min   | > 99                  |
| 5     | 1 mol% CuO-poly   | 100       | 10 min   | 27 <sup>c</sup>       |
| 6     | 0.5 mol% CuO-poly | 100       | 10 min   | 38                    |
| 7     | recovered # 4     | 100       | 10 min   | 99                    |
| 8     | recovered # 7     | 100       | 10 min   | 100                   |

<sup>a</sup> Determined by <sup>1</sup>H-NMR. Yields are based on the amount of benzyl azide used.

<sup>b</sup> Traditional stirring. <sup>c</sup> Conventional thermal heating at 100°C



일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: III-INOR.P-33

발표분야: 무기화학

발표종류: 포스터, 발표일시: 금 10:30~12:30

## Synthesis of Highly Soluble Anthraquinone Dichroic Dye in Liquid Crystal

김재현, 유찬용, \*이상근, \*\*서금석, 박강현

부산대 화학과 \*(주)제이피에스 마이크로텍 기업솔 연구소 \*\*(주) 제이피에스 마이크로텍 총괄

The application of liquid Crystal Display (LCD) has been immensely broaden recently due to its nature of excellent power efficiency while retaining full color display with high contrast. The color displayed is determined by mixing the amount of red, green and blue light that are produced with back light source and dichroic dye molecules. The key requirements for the effective dichroic dyes are color intensity, photo stability, and the solubility within the LC molecules. Anthraquinone dyes are known for the quality color along with the photo stability, yet the solubility is quite low that is between 1 and 3%. Controlling over the substituents of the anthraquinone dyes, we were able to synthesize more effective dichroic dyes with the solubility over 5%.

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장소: 제주ICC

발표코드: III-INOR.P-34

발표분야: 무기화학

발표종류: 포스터, 발표일시: 금 10:30~12:30

## CuO/AB 촉매를 이용한 Aryl-Sulfur Cross Coupling의 선택성 연구

변만수, 박강현

부산대 화학과

최근 다양한 크기와 모양, 서로 다른 구조의 나노 소재 개발을 통해 실용적인 가치가 있는 신 나노물질의 창출과 함께, 이를 산업화에 적용하려는 움직임이 있다. 따라서 우리는 나노촉매에 초점을 두고 기존의 반응방법이 아닌 Microwave 를 이용하여 반응을 하였다. Microwave 가 가지는 특징인 쉽고 빠르고 간단함은 온화한 조건(고온 또는 고압이 아닌 STP 의 상태)에서 반응을 가능하게 한다. 유기반응으로는 iodobenzene 과 thiophenol 의 cross coupling reaction 을 선택하였다. CuO 나노입자를 이용하여 용매 및 실험온도, 시간을 달리하여 연구한 결과 촉매 5 mol% CuO/Acetylene black, Microwave 반응온도 120 ℃, 반응시간 20 분, 용매 DMSO 일때 60% 수득율로 diphenylsulfane 의 선택성이 90%가 나왔다. 이러한 결과는 다양한 나노촉매의 이용가능성을 보여준다. 또한 다양한 Microwave 의 반응시간 및 온도변화를 통해 유기합성반응을 더욱 온화한 조건에서 높은 수득율로 얻을 수 있다는 결과를 제시해준다.

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## 마이크로웨이브를 이용한 비등방성 CuPt나노막대입자의 합성

김영수, 박강현

부산대 화학과

요즘 관심이 높아지고 있는 나노화학은 모양, 크기에 따라 특이한 성질을 가지고 있어 디바이스에서 대체 에너지원까지 다양한 분야에 응용가능하다. 마이크로파를 나노입자 합성에 이용함으로써 기존에 전통적인 나노입자 합성방법에서 벗어난 쉽고 빠르며 간단하게 우수한 질의 비등방성 CuPt 나노막대입자를 선택적으로 합성하였다. Platinum acetylacetonate , copper(II) acetylacetonate , 1,2-hexadecanediol, oleic acid ,oleylamine , 1-octadecene 를 넣고 120 ℃, 1000 W, 5 분으로 진행한 후 225 ℃, 1000 W, 10 분의 조건으로 반응시켰다. 그 결과 CuPt 가 평균 23 nm 의 막대입자로 합성되었고, 같은 합성온도에서도 시간을 달리함에 따라 CuPt 나노막대입자의 크기가 조금씩 달라짐을 알 수 있었다. 합성한 나노입자를 추가적인 분리과정없이 침전과 원심분리를 이용하여 쉽고 간편한 방법으로 나노막대입자만을 얻을 수 있었다. 추후 합성한 CuPt 나노막대입자를 유기반응의 촉매로 사용하여 그 효율성을 연구할 것이다.

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## A Novel Design Principle Towards Turn-On Phosphorescent Sensors for Fluoride

Ramesh Vadavi, 김태원, 성우영, 박성훈, 이민형

울산대 화학과

Fluoride anion is known for its harmful effects on humans and environment. As a result, various sensing techniques have been developed for the purpose of detecting fluoride ion. Efforts to develop fluoride ion sensors using triarylborane receptors have been accomplished based on absorption, colorimetric and fluorescence changes. Recently, the use of phosphorescent heavy-metal complexes as chemosensors has attracted considerable interest because of advantageous phosphorescent properties of heavy metal complexes. In this regard, we designed and synthesized new heteroleptic Ir(III) complexes  $[\text{Ir}(\text{C}^{\wedge}\text{N})_2(\text{LX})]$  (where  $\text{C}^{\wedge}\text{N}$  is ppy or btp and LX is 4-(dimesitylboryl)benzoate) and their fluoride adducts. It is found that both the complexes could be used as highly selective chemosensors for fluoride due to the interaction of a borane group on the LX ligand with fluoride. In particular, it is revealed that the complexes can act as Turn-On phosphorescent sensors towards fluoride. The details of synthesis, characterization, and photophysical properties of Ir(III) complexes and their fluoride complexation behavior will be presented.

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발표코드: III-INOR.P-37

발표분야: 무기화학

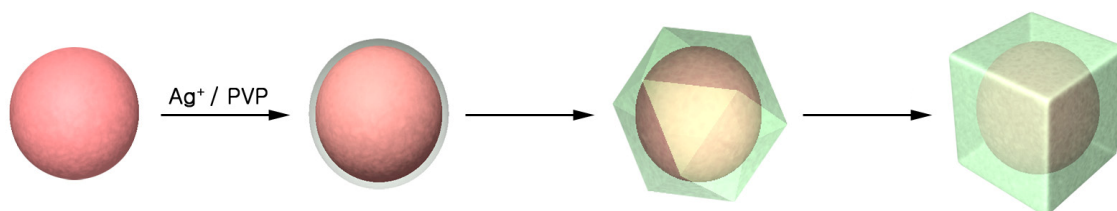
발표종류: 포스터, 발표일시: 금 10:30~12:30

## Shape Evolution and Gram-Scale Synthesis of Gold@Silver Core-Shell Nanopolyhedrons

박가람, \*류설, 송현준

KAIST 화학과 \*조선대 화학과

Bimetallic nanoparticles are currently of much interest because of their physical properties distinct from a simple combination of each metal component. Among bimetallic nanostructures, core-shell type nanoparticles have widely been studied in order to utilize multiple functionalities of independent domains. Gold and silver are representative noble metals and have similar lattice constants with a small lattice mismatch (0.2%), that leads to heteroepitaxial growth on the surface. Recently, Au@Ag heterometal core-shell nanoparticles with distinct polyhedral shapes were successfully synthesized by a seed-mediated polyol process in a gram scale. The addition of the silver precursor solution led to continuous shape evolution from gold seeds to silver spheres, cuboctahedrons, and cubes, respectively. Silver nanocubes were also grown by selective edge growth on gold cuboctahedral seeds. Because of distinct dielectric constants, gold and silver strongly scatter light in different wavelengths, and thus the overgrowth of silver shells on gold seeds could precisely tune the optical properties in the visible range. Interestingly, a large red-shift of the extinction peak from that of the gold seeds was observed in the Au cuboctahedron@Ag cubes, reflecting a combination of composition and shape effects.





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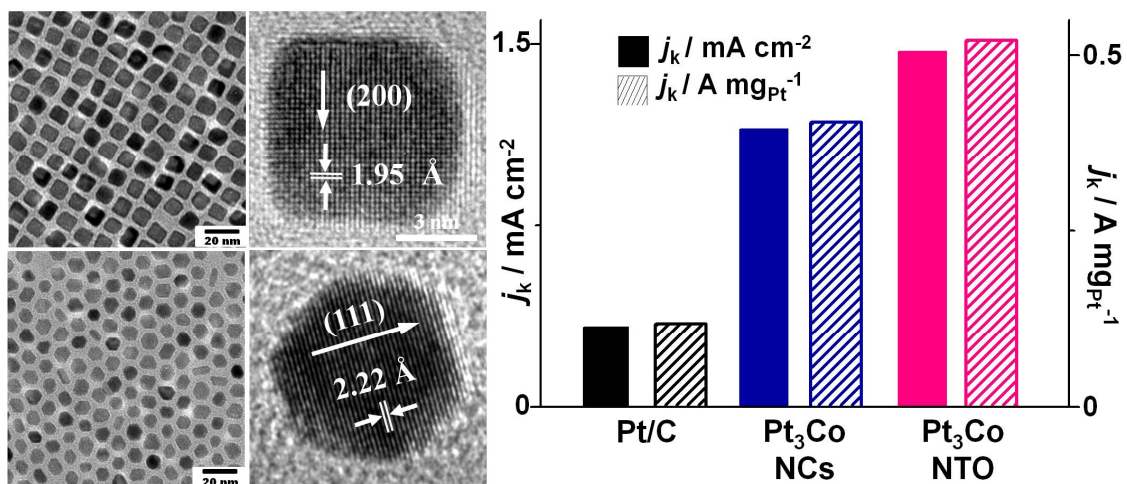
## Shape-Controlled Synthesis of Pt<sub>3</sub>Co Nanocrystals with High Electrocatalytic Activity toward Oxygen Reduction

최상일, 최란, 한상우, \*박준택

KAIST 화학과 \*한국기초과학지원연구원 원장실

Pt nanoparticles are the most efficient catalysts for the oxygen reduction reaction (ORR) at the cathode in a polymer electrolyte membrane fuel cell (PEMFC).<sup>1</sup> Important strategies for developing highly active Pt catalysts have included the control of the surface arrangements of the Pt particles and the use of Pt-based bimetallic particles in place of pure Pt as the electro-catalyst.<sup>2,3</sup> In these regards, the synthesis of Pt alloy nanocatalysts with controlled morphologies is one of the most critical issues for enhancement of their catalytic activities. Very recently, we have demonstrated that the Pt<sub>9</sub>Co alloy nanocubes bound by {100} planes show a 4-fold improvement of catalytic activity toward ORR than that of the commercial Pt/C catalyst in H<sub>2</sub>SO<sub>4</sub> solution.<sup>4</sup> Herein, we describe the synthesis of Pt<sub>3</sub>Co nanocubes (NCs) and nano-truncated octahedra (NTO) of which surfaces are dominated by {100} and {111}/{100}. The selective synthesis of Pt<sub>3</sub>Co NCs and NTO could be achieved by controlling the reaction time. Electrocatalytic experiments reveal the shape-dependent ORR activities and the significantly improved activity for Pt<sub>3</sub>Co NTO, showing that the specific facet of Pt<sub>3</sub>Co nanocrystal associated with its shape plays a determining role in the catalytic activity of the crystals. The present facile morphology control of catalysts might provide a promising strategy for the development of efficient cathode catalysts for PEMFCs.

References 1. B. C. H. Steele, A. Heinzel, *Nature* 2001, 414, 345. 2. C. Wang, H. Daimon, T. Onodera, T. Koda, S. Sun, *Angew. Chem. Int. Ed.* 2008, 47, 3588. 3. V. R. Stamenkovic, B. S. Mun, M. Arenz, K. J. J. Mayrhofer, C. A. Lucas, G. Wang, P. N. Ross, N. M. Markovic, *Nat. Mater.* 2007, 6, 241. 4. S.-I. Choi, R. Choi, S. W. Han, J. T. Park, *Chem. Comm.* 2010, 46, 4950.



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## Crystal structure and electronic properties of 2-amino-2-methyl-1-propoanol (AMP) carbamate

조은희, 최상범, 전영호, 김자현

승실대 화학과

A crystal structure of a carbamate of 2-amino-2-methyl-1-propoanol (AMP-carbamate) has been elucidated and its structural and electronic properties investigated by density functional theory calculations and natural bond orbital analyses. The AMP-carbamate, highly unstable in aqueous solution, can be isolated as a salt with a protonated AMP by the reaction of neat AMP with atmospheric carbon dioxide. NMR spectroscopic analyses showed the carbamate to be slowly hydrolyzed in dimethyl sulfoxide- $d_6$  when the solution is exposed to air. The AMP-carbamate has a larger rotational freedom for its  $-NCO_2-$  moiety than a carbamate of monoethanolamine. Furthermore, it possesses a unique hyperconjugation between a lone pair orbital of a nitrogen atom and a C-C antibonding orbital.

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## Facile synthesis of core-shell metal-organic frameworks

강은영, 오유진, 심재웅, 김자현

승실대 화학과

Core-shell metal-organic frameworks (CS-MOFs) can be prepared in a sequence, that is, a core MOF acts as a substrate for the hetero-epitaxial growth of a shell MOF. In an ideal case, each core MOF crystal having a uniform shape and size would be coated evenly by a shell MOF, which results in a CS-MOF that have a definite composition ratio between the core and shell MOFs. However, in fact, it is not easy to control both the shape and size of a core MOF during one-pot solvothermal reactions. To overcome this problem, instead of the step-by-step technique, we have devised a simple one-pot synthesis of CS-MOFs which requires a pH adjustment of a reaction mixture containing two kinds of metal ions and a bridging ligand. In the reaction, each metal ion has a different reactivity with a ligand, and therefore, after forming a core MOF, the second metal ion starts to form a shell MOF on the surface of the core. Using this facile method, we could make a series of square grid CS-MOFs with reaction mixtures containing two kinds of metal ions (for example, Cu/Zn or Cu/Co) and ditopic bridging ligand (NDC). Syntheses and characterizations of CS-MOFs will be presented with their pore properties.

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## Computations on the carbon dioxide absorption reactivity of linear and cyclic amines

전영호, 조은희, 김자현

승실대 화학과

Cyclic amines are known to react with CO<sub>2</sub> faster than linear amines. The reason is generally ascribed to the larger steric hindrance exerted by the flexible linear amines to incoming CO<sub>2</sub> than cyclic ones. In order to evaluate the accessibility of CO<sub>2</sub> toward amines, we carried out molecular dynamics simulation for the systems composed of amine, CO<sub>2</sub>, and H<sub>2</sub>O molecules, mimicking the real CO<sub>2</sub> absorption reaction media. The accessibility has been assessed by counting the number of van der Waals contacts between CO<sub>2</sub> and cyclic or linear amine observed during the MD simulation. Nucleophilicity of each amine was also calculated using DFT calculations. The absorption reactivity of both amines has been analyzed and interpreted based on the relationship between the nucleophilicity and accessibility.

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발표분야: 무기화학

발표종류: 포스터, 발표일시: 금 10:30~12:30

## Liquid Phase Synthesis and Controlled Growth Mechanism of GeTe Crystals

김명호, 김진권

공주대 화학과

Chalcogenide alloys exhibiting a thermally induced, reversible, amorphous-to-crystalline phase change are important for a wide range of technologies. Germanium telluride (GeTe) is simultaneously the phase change memory material and the ferroelectric material with the simplest composition. Solution routes are attractive alternative strategies for synthesizing these materials, because they have the potential to impart morphology control on the crystallites and permit liquid-based processing of films and patterned structures. Reactions carried out with Germanium(II) chloride dioxane complex and trioctylphosphine-tellurium (TOP-Te) in oleylamine(OLA) at 150°C yielded GeTe crystals. The GeTe crystals are characterized by SEM(scanning electron microscope), EDS(energy dispersive spectroscopy), TEM(transmission electron microscope), DSC(differential scanning calorimetry) and XRD(X-ray diffractometer). Interestingly SEM and TEM images show formation of nano size GeTe particles together with Te rods on Short reaction time(2min), whereas it shows formation of only GeTe crystal on long reaction time(1hr).

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발표분야: 무기화학

발표종류: 포스터, 발표일시: 금 10:30~12:30

## Liquid Phase Synthesis of GeTe Microparticles without any reducing agents

김명호, 김진권

공주대 화학과

Chalcogenide materials such as germanium telluride (GeTe:GT) have attracted a great deal of attention due to their reversible phase change properties which are used in the fields of optical data storage (CD and DVD) and phase-change random access memory (PRAM). Rhombohedral GeTe microparticles (MPs) were successfully synthesized without any reducing agents by solution-based process. Reaction carried out with Germanium(II) chloride dioxane complex,  $(\text{Et}_3\text{Si})_2\text{Te}$  in Trioctylphosphine oxide (TOPO) at  $250^\circ\text{C}$  yielded rhombohedral GeTe MPs. The GeTe MPs are characterized by SEM (scanning electron microscope), EDS (energy dispersive spectroscopy), TEM (transmission electron microscope), DSC (differential scanning calorimetry) and XRD (X-ray diffractometer). Scanning electron microscopy (SEM) images show formation of sphere shaped GeTe MPs. Rhombohedral GeTe MPs length of  $\sim 0.4 \pm 0.1 \mu\text{m}$ .

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발표분야: 무기화학

발표종류: 포스터, 발표일시: 금 10:30~12:30

## Synthesis and characterization of macrocyclic nickel(II) coordination polymers containing bridging ligands

신향진, \*한동완, \*류충도, 김주창

부경대 화학과 \*부산대학교

The chemistry of the coordination polymers constructed from metallomacrocycles and polycarboxylate ligands has been developed extensively due to a wide variety of potential applications such as catalysis, chirality, photochemistry, conductivity, and magnetism, etc. In this work, we will present the synthesis and structural characterization of nickel(II) coordination polymers containing nickel(II) macrocycles as “connectors” and bridging ligands as “linkers” to better understand the interactions between nickel(II) macrocycles and bridging ligands.



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발표종류: 포스터, 발표일시: 금 10:30~12:30

## Formation of Ge-132 nanofibers and their self-assembly into nanobelts in aqueous medium

이준, 모수용, 우희권

전남대 화학과

One-dimensional (1D) nanobelts of several hundred micrometers in length, several hundred nanometers in width and in height are obtained from Ge-132 aqueous solution at room temperature. The nanobelts were characterized by elemental analysis,  $^1\text{H}$  NMR, FT-IR, thermogravimetric analysis (TGA). The nanobelts are identified as Ge-132 assemblies. The formation of the nanobelts involves two stages: (1) hydrolysis of Ge-132 by proton, yielding individual Ge-132 molecules; and (2) self-assembly of the oligomeric Ge-132, forming the 1D nanobelts. The nanobelts exhibit fairly high thermal stability. In addition, uniform nanofibers have been successfully synthesized by incorporating Ge-132 with  $\text{H}_2\text{PtCl}_6$  under ambient conditions. Redox reactions between Ge-132 and  $\text{Pt}^{4+}$  ions, which result in the partial oxidation of Ge-132 should occur with simultaneous partial reduction of the metal ions  $\text{Pt}^{4+}$  to Pt. The  $\text{Pt}^{4+}$  and Pt ions can coordinate with  $(\text{C}=\text{O})\text{O}^-$  functional groups of Ge-132 should introduce the formation the 1D nanostructure. The size and morphology of the nanofibers can be easily controlled by tuning the molar ratio of Ge-132 and  $\text{H}_2\text{PtCl}_6$  and their initial concentrations.

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발표분야: 무기화학

발표종류: 포스터, 발표일시: 금 10:30~12:30

## Growth Mechanism for t-Selenium Nanotubes: Solution-Phase Synthesis and Molecular Orbital Calculation

이준, 김종현, 우희권

전남대 화학과

We report a wet-chemical reaction to make t-selenium nanotubes, in the absence of a surfactant or polymer to direct nanoparticle growth, without external forces (such as ultrasonic activation). The selenium nanotubes were directly prepared using Se powder as selenium source by mild solution method. The synthetic reaction was carried out with cellulose as both reducing and morphology-directing agents in aqueous solution under simple conditions at room temperature, which is quite different from the thermal evaporation/reaction process for nanotubes at high temperature. A series of electron microscopic characterization results suggest that the growth of t-selenium nanotubes is governed by a nucleation-dissolution-recrystallization growth mechanism. As-prepared t-selenium nanotubes may possess unique electronic properties. The electronic properties of selenium crystals were investigated using molecular orbital calculations (GAUSSIAN03). It was found from the results that the growth mechanism is strongly affected by both temperature and concentrations of reactants. Therefore, by adjusting temperature and concentrations of reactants, t-selenium nanotubes, nanowires, nanorods, and porous microtubes can be synthesized, respectively.

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발표분야: 무기화학

발표종류: 포스터, 발표일시: 금 10:30~12:30

## Synthesis of Pt-Tipped CdSe hybrid structures for Photocatalytic Hydrogen Generation under visible light

방정엽

KAIST 화학과

The photocatalyst which can operate under visible light is a promising route for harnessing of solar energy to convert to light to chemical energy. Semiconductors and metal-semiconductor hybrid structures have been studied as photocatalysts in photochemical water splitting to produce hydrogen. Many metal oxides such as  $\text{TiO}_2$  and  $\text{ZnO}$  are known to catalyze the water splitting reaction, but their bandgaps are suitable only to absorb the UV range, which consists of less than 5% of the solar spectrum. Moreover, the degree of control over particles size and shape was limited. We synthesized highly controlled Pt tipped CdSe hybrid nanostructure which can operate under visible light as a photocatalyst. Under visible light irradiation, this highly controlled structure show high activity for water splitting reaction.

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발표분야: 무기화학

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## Synthesis of Organo-copper Complexes and Their Conducting Ability in the Paste and Inks

구자민, \*이병철, \*\*박지현, \*\*\*이효선

경북대 화학과 \*한국원자력연구소 양자광학연구부 \*\*과학기술연합대학원대 레이저및플라즈마  
응용공학 \*\*\*경북대 자연과학대학 화학과

Conductive materials have been extensively researched due to their inevitability for electronic industry over the past few decades. In order to prepare conductive patterns with improve cost/performance characteristic, a conductive copper ink as an alternate substance is thus configured. This process has been successfully achieved via thermal treatment or other electromagnetic radiation with the ease of its operation, economical and environmentally friendliness coupled with the preventing ability of Cu oxidation. To obtain the paste or ink composed of copper metal, the Cu ligation with N-methyldiethanol amine, N-triethanol amine, 3-[Bis-(2-carboxy-ethyl)-amino]-propionic acid, terephthalic acid, and glutaric acid by thermal heat and ultrasonics, has been carried out. Moreover, new the copper complexes supported by thiophene and its derivative was further synthesized. All complexes were prepared in high yield, and well characterized to be exploited for conductive pastes and inks.

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## Synthesis and Characterization of Non-Cp Based Titanium-hydrocarbyl Complexes for $\alpha$ -Olefin Polymerization

우현율, \*이동민, \*\*이효선

경북대 자연과학대학/화학과 \*경북대 화학과 \*\*경북대 자연과학대학 화학과

Dialkyl titanium and zirconium complexes such as  $L_2TiR_2$  ( $R = Me, CH_2Ph$  etc.) have been known for isolable key intermediate for  $\alpha$ -olefin polymerization in the presence of cocatalyst, for example, trialkylborane and tetraalkylborate. Thus, their chemistry have been extensively reported and studied as non-Cp metallocene complexes for an olefin polymerization. Here we report new dihydrocarbyl complexes,  $LnTiR_2$  ( $R = Me, CH_2Ph, CH_2SiMe_3, Ph$ ) which is ligated to either  $L1$  or  $L2$  where ( $L1 = [OCH_2CH_2]_2NMe$ ,  $L2 = [CH_2SiMe_3]_2$ ). The synthesized complexes was investigated for their catalytic (co)polymerization ability toward olefins such as ethylene and cyclic olefin norborne using MMAO or trialkylaluminum as a cocatalyst.

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발표분야: 무기화학

발표종류: 포스터, 발표일시: 금 10:30~12:30

## Synthesis and Characterization of New Organometallic Complexes with New Ligand Base on ML-10 for Molecular Imaging and Therapy Agent

양민균, \*박상현, \*\*이효선

경북대 화학과 \*한국원자력연구원 방사선생명공학연구부 \*\*경북대 자연과학대학 화학과

Apoptosis plays an important role in normal tissue homeostasis and in pathogenesis of numerous medical disorders. ML-10 responds to a unique complex of features of the cell in early apoptosis, comprising irreversible loss of membrane potential, permanent acidification of cell membrane and cytoplasm, and preservation of membrane integrity. ML-10 is amenable to radiolabeling with the  $^{18}\text{F}$  isotope, towards its potential future use for clinical positron emission tomography imaging of apoptosis. The clinical molecular imaging of this process may enhance diagnosis, efficiency of treatment, and monitoring of disease. Two methodologies were intended to use for the synthesis of new molecular imaging substrate system based on original ML-10 with the modification of fluoride moiety with several new tridentate ligands e.g. 2-[(pyridin-2-ylmethylene)-amino]-phenol, 2-[(bis-pyrazol-1-ylmethyl-amino)-methyl]-phenol, and carboxymethyl-amine coupled with the direct ligation of radiopharmaceuticals metals e.g.  $^{188}\text{Re}$ ,  $^{99\text{m}}\text{Tc}$  to nitrogen based ligand systems such as 2-[(pyridin-2-ylmethylene)-amino]-phenol, and Tris-(3,5-dimethyl-pyrazol-1-ylmethyl)-amine and Benzyl-bis-(3,5-dimethyl-pyrazol-1-ylmethyl)-amine, N,N-Bis{(1-H-Pyrazole-1-yl)methyl}aniline, N,N-Bis{(1-H-Pyrazole-1-yl)methyl}-2,4,6-trimethylaniline, N,N-Bis{(1-H-Pyrazole-1-yl)methyl}2,6-diisopropylaniline and N,N-Bis{(3,5-dimethyl-1H-pyrazol-1-ylmethyl)-2,6-diisopropylaniline. Furthermore, from application point of view the radioactive nature of the metal in the synthesized complexes can be exploited as a therapy agent and for labeling biomolecules for treatment of the cancer affected cells as well as in clinical molecular imaging for monitoring the cancer affected cell response to treatment and the efficiency of treatment as these compounds respond to the alteration in plasma membrane potential. Furthermore, the beta rays emitted energy for treatment of cancer cell directly is under investigation.

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발표분야: 무기화학

발표종류: 포스터, 발표일시: 금 10:30~12:30

## **Tubular microporous networks bearing imidazolium salts and their catalytic CO<sub>2</sub> conversion to cyclic carbonate**

이한솔, 손성욱

성균관대 화학과

Catalytic CO<sub>2</sub> conversion to other organic forms is an important subject due to environmental concerns. Diverse organic reaction partners such as amines, alcohols and hydrogen can be used to transform CO<sub>2</sub> into carbamates, bicarbonates and alcohols, respectively. Among the diverse transformations, the formation of cyclic carbonates via reaction of CO<sub>2</sub> with epoxides have attracted continuous attention because the resultant products can be used as solvents or raw materials for industrial production of polycarbonates. Recently, for more convenient separation of cyclic carbonates from catalytic systems, heterogeneous solid catalysts with supported imidazolium salts have attracted the attention of scientists. As a recent example, Han and co-workers prepared promising non-porous heterogeneous systems by polymerization of divinylbenzene and vinyl imidazolium salts. However, efficient catalytic systems based on ammonium salts are still quite limited and more exploration is required, especially for higher turnover frequencies (TOFs). Our research group has studied functional materials bearing imidazolium salts or relevant N-heterocyclic carbenes (NHCs). In this presentation, we introduce the designed synthesis of porous and tubular organic networks bearing imidazolium salts (T-IM) and their heterogeneous catalytic activities in CO<sub>2</sub> conversion to cyclic carbonates.

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발표분야: 무기화학

발표종류: 포스터, 발표일시: 금 10:30~12:30

## Synthesis, Structural Characterization, and Heteroselective Polymerization of rac-Lactide by Chiral Dimethyl Zinc complexes supported by [(S,S)-1-Phenyl-ethyl)-pyrrolidin-2-yl-amine] and its Derivatives

Navab Saira, 정종화, \*이효선

경북대 화학과 \*경북대 자연과학대학 화학과

The attractive physical and mechanical properties of the polylactide (PLA) lend them to having numerous applications in medical, agriculture, and microelectronic areas. A series of new zinc dichloro complexes ligated by bidentate homochiral [(S,S)-1-Phenyl-ethyl)-pyrrolidin-2-yl-amine] and its alkyl derivatives have been synthesized in high yield and purity. The synthesized complexes were fully characterized by various spectroscopic techniques coupled with the crystal structure determination of dichloro [(S,S)-1-(6-methylpyridin-2-yl)-N-(1-phenylethyl)ethanamine] Zn (II) and dichloro [(S,S)-1-Phenyl-ethyl)-pyrrolidin-2-yl-amine] Zn (II) complexes. The catalytic capacity for Ring Opening Polymerization (ROP) of rac-Lactide was evaluated at two different temperatures. The active catalyst species was generated in situ by treating air and moisture stable dichloro Zn complexes with MeLi. The metal complex was found to be highly active for ROP of rac-lactide and the heterotactic PLA with Pr up to 89% was obtained by initiating polymerization in CH<sub>2</sub>Cl<sub>2</sub> at -23 °C. Furthermore, the thermal behavior and molecular weight of the obtained polymer was determined by DSC and GPC, respectively.



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발표분야: 무기화학

발표종류: 포스터, 발표일시: 금 10:30~12:30

## Ring Opening Polymerization of rac-Lactide Initiated by In-situ Generated Dimethyl Zinc Complexes Based on (R,R)-1,2-Diaminocyclohexane Ligand

Nayab Saira, 정종화, \*이효선

경북대 화학과 \*경북대 자연과학대학 화학과

New zinc complexes based on bidentate (N,N'-dibenzyl-(R,R)-1,2-diaminocyclohexane and its methoxy derivatives, on the phenyl group of benzyl moieties, have been synthesized and the crystal structures of the dichloro [N,N-bis(3-methoxybenzyl)-(R,R)-1,2-diaminocyclohexane] Zn (II) was determined by x-ray crystallography. The well characterized complexes were employed as an initiator for Ring Opening Polymerization (ROP) of rac-Lactide. The complexes were found to be highly efficient initiator yielding isotactic PLA with well molecular control and narrow molecular weight distribution. Experimental results indicate that the electronic effect of methoxy substituent's on the phenyl groups of benzyl moieties of (R,R)-1,2-diaminocyclohexane fragment has a dramatic effect on the stereoselectivity of the obtained PLA. Furthermore, the isotactic PLA with Pm up to 80 % can be obtained by initiating ROP of rac-lactide with in situ generated dimethyl zinc complexes in CH<sub>2</sub>Cl<sub>2</sub>. The molecular weight of the polymer was determined by GPC.

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발표종류: 포스터, 발표일시: 금 10:30~12:30

## A Facile Synthesis of Copper Oxide Nanowire Anodes for Lithium-Ion Batteries

이정인, 박수진

울산과학기술대 에너지공학부

과학기술의 발전과 함께 지금 사용 하고 있는 재료보다 우수한 성능과 새로운 기능을 갖는 재료의 개발이 필요하게 되었고, 이러한 요구를 만족하는 수에서 수십 나노미터의 크기를 갖는 물질의 개발이 요구되고 있다. 그 중, 나노와이어의 물리/화학적 성질을 이용하여 전자장비, 광학장비, 촉매 그리고 화학적 센서 등 다양한 영역으로 응용분야를 넓혀가고 있다. 본 연구는 수열합성법(hydrothermal process)을 통하여 합성되는 구리 나노와이어(copper nanowires)에 관한 것이다. 염화구리( $\text{CuCl}_2$ ) 또는 황산구리( $\text{CuSO}_4$ ) 수용액과 긴 알킬기(Long alkyl group)를 가지는 아민(Amine)계열의 물질( $\text{R-NH}_2$ ,  $\text{R}=\text{CH}_3(\text{CH}_2)_n$ ,  $n=9, 11, 13, 15, 17$ )을 반응시켜 구리 나노와이어를 합성한다. 또한 합성된 구리 나노와이어를 일정시간 동안 산소 분위기에서 열처리를 하면 Kirkendall effect 에 의하여 산화구리 나노튜브 (Copper oxide nanotubes)로 전환되고 이것은 리튬 이차 전지(Lithium-ion battery)의 음극 활물질로 이용될 수 있다. 본 연구의 수열합성법을 이용하여 합성되는 구리 나노와이어는 기존의 기술로 합성되는 구리 나노와이어 보다 합성방법이 쉽고 간단하며, 합성 시 사용되는 물질의 종류, 양, 반응 온도와 반응 시간 등 간단한 조작으로 구리 나노 와이어의 지름, 길이 그리고 모양을 쉽게 조절 할 수 있다.

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발표코드: III-INOR.P-55

발표분야: 무기화학

발표종류: 포스터, 발표일시: 금 10:30~12:30

## Synthesis, crystal structure, and magnetic properties of transition metal complexes ( $\text{Mn}^{\text{II}}$ , $\text{Co}^{\text{II}}$ , and $\text{Fe}^{\text{II}}$ ) with bis(4-pyridyl)benzylamine

로투산카라라오, 신종원, 김승휘, \*조현정, \*민길식

경북대 화학과 \*경북대 사범대학 화학교육과

The search for molecular materials exhibiting interesting properties such as bistability and magnetic ordering is a very challenging quest in the field of inorganic and coordination chemistry. A lot of work has been devoted to the study of exchange interactions between transition metal ions through extended bridging groups for elucidation of the fundamental understanding of the long-range magnetic interactions. Due to the interest we have synthesized manganese(II), cobalt(II), and iron(II) complexes with a bis(4-pyridyl)benzyl amine (bpba),  $[\text{Mn}(\text{bpba})_2(\text{NCS})_2] \cdot 3\text{H}_2\text{O}$  (1),  $[\text{Co}(\text{bpba})_2(\text{NCS})_2] \cdot 2\text{H}_2\text{O}$  (2), and  $[\text{Fe}(\text{bpba})_2(\text{NCS})_2] \cdot 2\text{CH}_3\text{OH} \cdot \text{H}_2\text{O}$  (3) from the reaction of  $[\text{Mn}(\text{H}_2\text{O})_6](\text{ClO}_4)_2$ ,  $[\text{Co}(\text{H}_2\text{O})_6](\text{NO}_3)_2$ ,  $[\text{Fe}(\text{H}_2\text{O})_6](\text{ClO}_4)_2$ , bis(4-pyridyl)benzylamine, and NaSCN in methanol under aerobic condition for 1 and 2 and under nitrogen for 3. In this presentation, the detailed preparation, crystal structure, magnetic properties of 1, 2, and 3 will be described.

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발표분야: 무기화학

발표종류: 포스터, 발표일시: 금 10:30~12:30

## Tunable Rhombus of Palladium(II) Complexes

안정민, 김은지, 정옥상

부산대 화학과

Metallacyclodimeric rhombus,  $[(\text{tmeda})\text{Pd}(\text{L})]_2(\text{CF}_3\text{SO}_3)_4$ , via the reaction of  $(\text{tmeda})\text{Pd}(\text{CF}_3\text{SO}_3)_2$  ( $\text{tmeda} = N,N,N',N'$ -tetramethylethylenediamine) with 1,3-bis(4-pyridyl)tetramethyldisiloxane (L) in acetone solution was crystallized via slow diffusion of co-solvents such as *n*-hexane, tetrahydrofuran, and 1,4-dioxane to yield single crystals containing each solvate molecules. The similarity and difference of the crystal structures were discussed based on X-ray single crystallography, IR,  $^1\text{H}$  NMR, and thermal data. The molecular metallacyclic rhombuses are delicately dependent on solvent. To the best of our knowledge, for *n*-hexane, this is unusual example to trap an aliphatic hydrocarbon in a host component.

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장소: 제주ICC

발표코드: III-INOR.P-57

발표분야: 무기화학

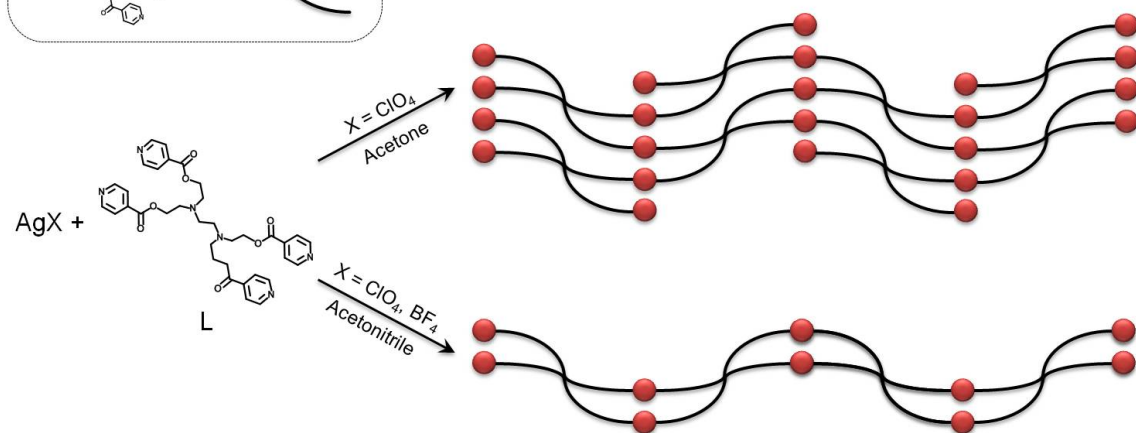
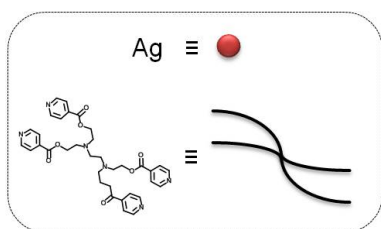
발표종류: 포스터, 발표일시: 금 10:30~12:30

## **Influence of Acetonitrile on Silver(I) complexes containing New Tetrakis(pyridyl) Ligand**

이소정, 정옥상

부산대 화학과

We report herein the synthesis of new potentially hexadentate ligand (L) and the crystal structures of silver(I) complexes containing the ligand. Self-assembly of  $\text{AgClO}_4$  with L yields 2-D coordination polymer consisting of  $[\text{Ag}_2(\text{L})](\text{ClO}_4)_2$ , that the ligand is as a spacer along with  $\mu_4$ -fashion, in a mixture of acetone and  $\text{H}_2\text{O}$  to solve using X-ray crystallography. Otherwise, vapor diffusion of diethyl ether into the saturated acetonitrile solution of the above compound leads to single crystals consisting of 1-D coordination polymers of same components except for additional acetonitrile along with intramolecular  $\text{Ag}\cdots\text{Ag}$  and  $\pi\cdots\pi$  interactions. According to the bond length and thermal stability, the acetonitrile is as a coordinating ligand rather than solvated solvent. That is, the coordination of additional ligand prevents the dimension of the structure from expand. Such a result may be ascribe to subtle combination of non-covalent interactions. Also, recrystallization via vapor diffusion of diethyl ether into the acetonitrile solution of  $[\text{Ag}_2(\text{L})](\text{BF}_4)_2$ , yields the similar results.



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발표분야: 무기화학

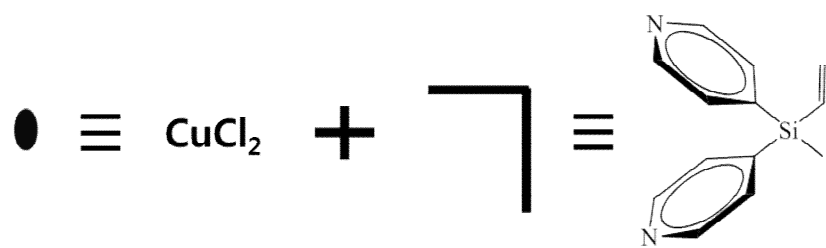
발표종류: 포스터, 발표일시: 금 10:30~12:30

## Helical Structures of Copper(II) Complexes Containing New Bis(4-pyridyl)methylvinylsilane Ligand

박경환, 정옥상

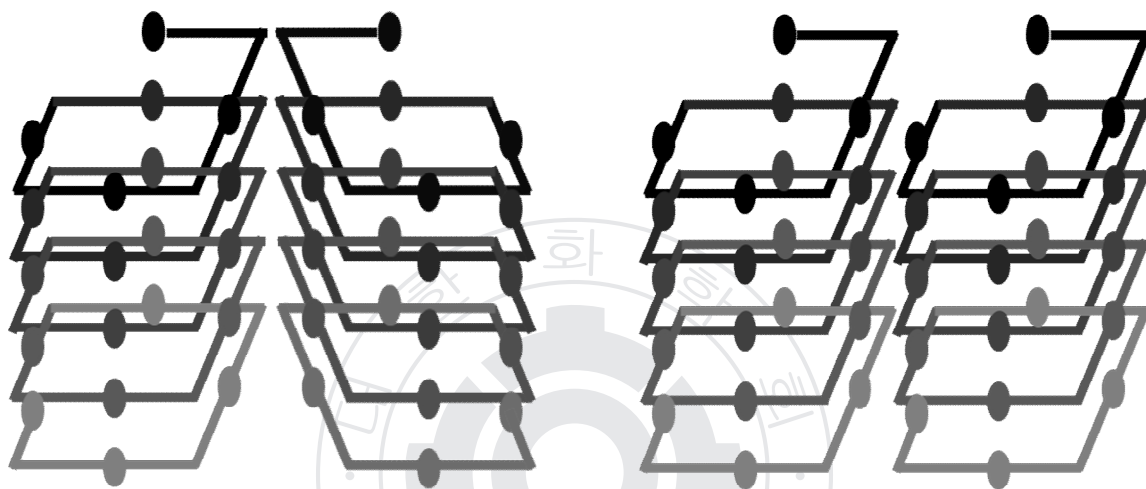
부산대 화학과

The reaction of  $\text{CuCl}_2$  with L (bis(4-pyridyl)methylvinylsilane) in a mixture of methanol and ethanol produces a greenish yellow precipitate. Vapor diffusion of diethyl ether into the *N,N*-dimethylformamide solution of the resulting solid yields single crystals consisting of racemic helical skeletal structure,  $[\text{CuCl}_2(\text{L})(\text{DMF})]$ , whereas vapor diffusion of ethyl acetate into the dimethylsulfoxide solution forms single crystals consisting of right-handed helical structure,  $[\text{CuCl}_2(\text{L})(\text{DMSO})]$ . Crystallographic characterization (solvent = DMF, cubic  $I-43d$ ,  $a = 30.848$  (4) Å,  $\beta = 90^\circ$ ,  $V = 29354$  (6),  $V = 29354$  (6) Å<sup>3</sup>,  $Z = 38$ ; solvent = DMSO, tetragonal  $P4_1$ ,  $a$  and  $b = 12.0021$  (7),  $c = 15.8352$  (10),  $\beta = 90^\circ$ ,  $V = 2281.1$  (2) Å<sup>3</sup>,  $Z = 4$ ) reveals that solvents play an important role in the construction of helices.



DMF

DMSO





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발표분야: 무기화학

발표종류: 포스터, 발표일시: 금 10:30~12:30

## Fabrication of $\text{CuInS}_2$ / $\text{ZnS}$ Quantum Dots by Cation Exchange

김태훈

아주대 분자과학기술학과

양이온 교환 반응을 이용하여 양자효율 65%를 가지는  $\text{CuInS}_2$  / $\text{ZnS}$  (CIS/ $\text{ZnS}$ ) 코어/셸 양자점을 합성하였다. 전자현미경을 통해 코어와 코어/셸 구조의 양자점 크기가 거의 같다는 것을 확인 하였다. 이를 통해, 코어의 크기가 줄어들었다는 것을 확인 하였으며, 이러한 이유 때문에 코어/셸 구조 합성 시 형광의 청색이동이 일어난다는 것을 확인 하였다. 또한 ICP 분석을 통해 합성된 CIS 코어의 조성이 중심부에는 구리 원소가 많고, 가장자리로 갈수록 인 원소가 많아진다는 것을 확인 하였다.  $\text{AgInS}_2$  (AIS) 도 합성하여 같은 방법으로 코어/셸 구조의 양자점을 합성하였으며, 이 또한 같은 원리로 인해 70nm 의 형광 청색이동을 관찰할 수 있었다.

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장소: 제주ICC

발표코드: III-INOR.P-60

발표분야: 무기화학

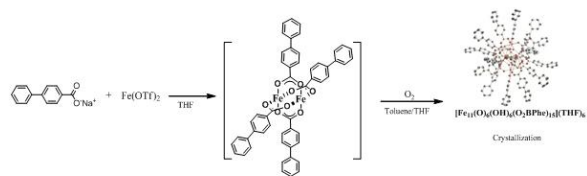
발표종류: 포스터, 발표일시: 금 10:30~12:30

## **Synthesis and Structure of a Carboxylate-Protected Iron-oxide Nanoparticle: Information on the Surfactant Binding on the Surface and Inter-digitation of Intra-Nanoparticle's Surfactants**

송혜선, 윤성호

국민대 생명나노화학과

Detailed structural information on the surface of surfactant-protected metal oxide nanoparticles(NPs) has been limited due to the difficulties of preparing the single crystal of nanoparticles suitable for the single crystal x-ray diffraction analysis. Herein, we report the synthesis and X-ray structural analysis of (C<sub>6</sub>H<sub>5</sub>)C<sub>6</sub>H<sub>4</sub>CO<sub>2</sub>H-protected iron oxide NPs, which comprises of 11 Fe(III) ions, 6 O<sup>2-</sup> atoms, 6 (OH-) ions and 15 C<sub>5</sub>H<sub>5</sub>C<sub>5</sub>H<sub>4</sub>COO- ions. The deprotonated surfactant, C<sub>5</sub>H<sub>5</sub>C<sub>5</sub>H<sub>4</sub>COO-, bridged the adjacent two Fe<sup>3+</sup> ions and the dissociated proton from the surfactant is located on the oxygen atom in Fe-O-Fe motifs, resulting in Fe-(OH)-Fe units. In addition, the intercalation between phenyl groups on the surface of the NPs is observed. Acknowledgements: This work was supported by the Korea Science and Engineering Foundation(KOSEF) grant funded by the Korea government (MEST) (R11-2005-048-00000-0)



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발표분야: 무기화학

발표종류: 포스터, 발표일시: 금 10:30~12:30

## Carbonic anhydrase models are linked on the surface of nanoparticles

김지연, \*윤성호, \*임상규, \*심진숙, \*\*최지은

국민대 화학과 무기화학전공 \*국민대 생명나노화학과 \*\*국민대 임산생명공학과

In recent years, the CO<sub>2</sub> capture and storage technology (Carbon Capture and Storage, CCS) to reduce greenhouse gas are of interest. Carbonic anhydrase is an enzyme with the essential role of catalyzing the reversible hydration of carbon dioxide. In the core of this enzyme, three N-donor ligands coordinated to a monomeric zinc cation play a key role. There are very few compounds, which can convert carbon dioxide to bicarbonate efficiently with monomeric zinc complex. Currently, we aim to synthesize new zinc complexes to mimic the carbonic anhydrase system with dipicolylamine or BBA moieties. Herein, our approaches in modeling the carbonic anhydrase system using organic/inorganic synthesis and sequential application to the CCS technology are presented. 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)

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발표분야: 무기화학

발표종류: 포스터, 발표일시: 금 10:30~12:30

## Fabricating Transparent Conductive Films with the Length Controlled Ag Nanowires

주본식, \*윤성호

국민대 화학과 \*국민대 생명나노화학과

Transparent Conductive Films(TCF) are used in a wide variety of applications, including low-emissivity windows, flexible displays, touch panels, and thin-film solar cells. Many companies prefer to use Indium-Tin Oxide (ITO) as the TCF because it can be applied at relatively low temperatures compared to other conducting oxides, and it's easier to etch than materials with comparable conductivities and transmittances. ITO films with a sheet resistance of  $10\Omega/\square$  transmit about 90% of visible light. Limitations of ITO include that it is brittle, and thus it cannot be used in flexible displays. And weakness of ITO is increasing that price, as consumption of TCF rapidly increase. Many group focus to find the alternative and inexpensive way to fabricating TCF. There are some emerging alternatives, such as single-walled carbon nanotubes(CNT), graphenes, metal, and metal nanowires. Recently, Yi Cui group have shown flexible TCF of silver nanowires have conductivities and transmittances comparable to ITO. This flexible TCF have a sheet resistance of  $20\Omega/\square$  transmit about 80 % of visible light. <sup>[1]</sup> TCF of silver nanowires has less efficient than ITO films. We must improve the TCF of silver nanowires in order to use it in future. We assume if the length of silver nanowires increase, the efficiency of TCF fabricated silver nanowires are also increased. We synthesized silver nanowires that they have different length, through controlled injection rate from 0.3 mL/min to 0.05 ml/min. And then, we fabricated TCF of silver nanowires having different length. The TCF of silver nanowires are characterized by UV-Vis, sheet resistor, and SEM.[1] Liangbing Hu, Han Sun Kim, Jung-Yong Lee, Peter Peumans, and Yi Cui, ACS Nano, 2010, 4, 2955 Acknowledgement: This work was supported by the Korea Science and Engineering Foundation(KOSEF) grant funded by the Korea government (MEST) (R11-2005-048-00000-0)

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발표분야: 무기화학

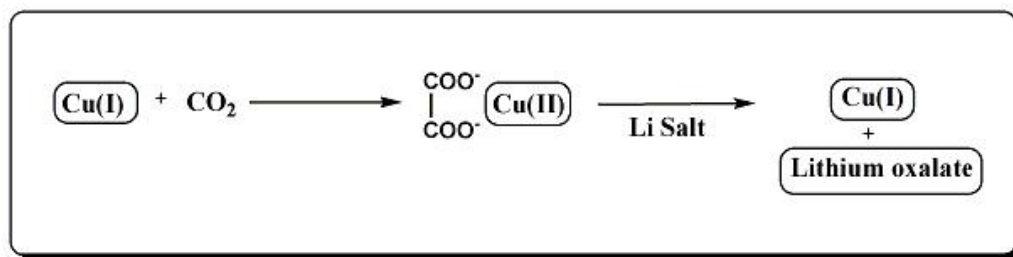
발표종류: 포스터, 발표일시: 금 10:30~12:30

## **Carbon dioxide was used as feedstock to synthesis oxalate by a copper (I) complex**

**D.Sivanesan, \*윤성호**

국민대 화학과 \*국민대 생명나노화학과

Reductive fixation of carbon dioxide into a useful organic compound is of interest as a result of alarming reports linking global warming and energy crisis. Transition-metal complexes, especially of copper and zinc, are well known for their assistance in the stoichiometric transformation of carbon dioxide to carbonate salts. In contrast, reductive conversion of CO<sub>2</sub> into useful products of industrial significance such as formaldehyde, formic acid, methanol, or oxalic acid has proven more challenging to achieve selectively. Herein, we report the synthesis of a new copper(I) catalyst and its reactivity toward the carbon dioxide. 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 (2010-0012349)



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발표분야: 무기화학

발표종류: 포스터, 발표일시: 금 10:30~12:30

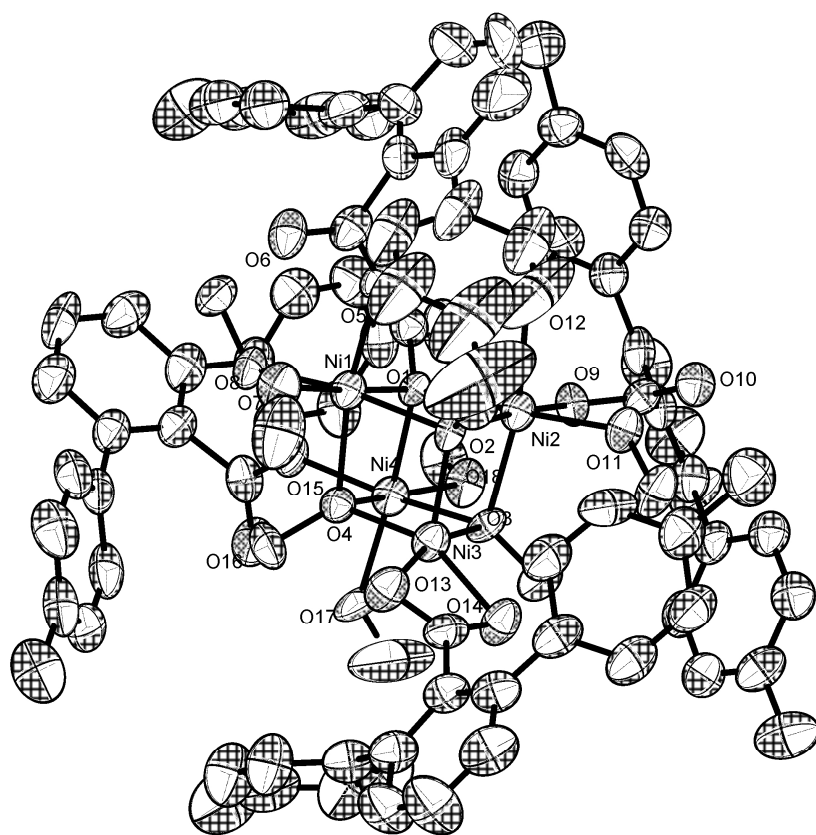
## The steric hindrance of carboxylate ligands triggers the change of coordination number of metal centers in cubanes

김남석, 윤성호

국민대 생명나노화학과

The metal coordination geometry in the active site of metalloproteins are very different from the one of small inorganic complexes, due to the inflexibility of the ligand set from amino acid side chains different from freely moving ligand set in synthesis. Among the richness of coordination chemistry, polynuclear metal complexes have focused an intense interest due to their potential involvement in biological systems. For example, some polynuclear metal complexes are good synthetic models for iron-sulfur proteins or photosystem II(PS II), mostly based on cubane-like architectures. Recently, a series of cubane Mn(II), Fe(II), Ni(II) complexes of general formula  $[M_4(\mu\text{-OMe})_4(L)_4(\text{MeOH})_8]$  and  $[M_4(\mu\text{-OMe})_4(L)_4(\text{MeOH})_6]$  have been synthesized using sterically hindered 2,6-di-(p-methylphenyl)benzoate and 2,6-di-(p-fluorophenyl)benzoate ligands. Herein the synthesis and characterization of cubane (Mn, Fe, Ni) complexes with the 6 and 5 coordination numbers of the metals are presented. 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)





HEAN CHEMICAL

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발표분야: 무기화학

발표종류: 포스터, 발표일시: 금 10:30~12:30

## Study of Emission Properties of Graphene and Lanthanide-mixtures

오영희, 최은주, 강보배, 홍성국, 김경안

동의대 화학과

Photoluminescent graphene/lanthanide(III) nanostructured materials have been prepared from the graphene,  $\alpha$ -pyridoin and Eu(III) and Tb(III) mixture in alcoholic solution in different ratios of metals. Photoluminescent properties of the materials were examined for the materials. Europium red emission has been changed to terbium green emission as the increasing of Eu/Tb ratios in the same reaction bottle. Emission of white light can be observed by carefully designed systems with the ratio of metals.

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발표분야: 무기화학

발표종류: 포스터, 발표일시: 금 10:30~12:30

## Synthesis and characterization of spinel $\text{Li}_4\text{Ti}_5\text{O}_{12}$ anode material by agarose template

홍태은, \*백성림, \*정옥상, 정의덕

한국기초과학지원연구원 부산센터 \*부산대 화학과

Spinel  $\text{Li}_4\text{Ti}_5\text{O}_{12}$  are becoming the promising negative electrode materials because of excellent Li-ion intercalation potential, cyclability and rate capability for lithium ion batteries. In this study, The  $\text{Li}_4\text{Ti}_5\text{O}_{12}$  was successfully synthesized using the agarose template. An agarose gel is ideal templates for the sol-gel synthesis of porous metal oxide structure. We obtained  $\text{Li}_4\text{Ti}_5\text{O}_{12}$  samples with different specific surface areas by variation of the agarose content. The crystal structure and morphology of synthesized  $\text{Li}_4\text{Ti}_5\text{O}_{12}$  have been investigated. We present the structural and electrochemical characteristics of spinel  $\text{Li}_4\text{Ti}_5\text{O}_{12}$  materials

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발표분야: 무기화학

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**Synthesis of InP/ZnS nanocrystal quantum dots using new phosphorus precursor: Optical and structural characterization**  
**SoMyoung Joung, SungWoo Yun, YoungJo Kim, and Sohee Jeong**

정소명

충북대 화학과

Semiconductor nanocrystal quantum dots(NQDs) have attracted attention as they can be applied in various areas such as LED, biological imaging, solar cell, and so on. For them to be of practical value, there is a need for a method that provides rapid and scalable production of highly monodispersed nanoparticles. We present a new synthetic scheme for the preparation of InP nanocrystal quantum dots using new phosphorus precursor. InP nanocrystals from 530nm to 600nm have been synthesized via the reaction of  $\text{In}(\text{Ac})_3$  and new phosphorus precursor in noncoordinating solvent, ODE. The nanocrystals are highly crystalline, monodisperse, and soluble in various organic solvent.

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발표분야: 무기화학

발표종류: 포스터, 발표일시: 금 10:30~12:30

## **Synthesis of Mesoporous Silica Materials with Core/Shell Structure And Their Catalytic Activity**

정경화

아주대 분자과학기술센터

We synthesized mesoporous shell silica bead (MSHS, Mesoporous SHell Silica bead) with dense silica core and porous silica shell. For the catalytic activity, MSHS was functionalized with sulfonic acid and aluminium, respectively and was tested by dehydration reaction of d-xylose into furfural. Sulfonic acid modified MSHS was higher selectivity of furfural than that of aluminosilicate MSHS. Also, MSHS is a efficient catalysis system in dehydration of gycelin. Finaly, We suggest that MSHS will be a frendly catalyst in field of dehydration under water system.

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발표분야: 무기화학

발표종류: 포스터, 발표일시: 금 10:30~12:30

## Synthesis of Zinc-chalcogenide nanoparticles through a simple sonochemical method

송미연, 황차환, 정원목, 심일운

중앙대 화학과

Colloidal II-VI semiconductor nanoparticles(NPs) are of great interest for fundamental studies(i.e., quantum size effects) and because of their promising applications in the field of light-emitting diodes(LEDs), lasers, solar cells, gas sensors, chemical sensing, and biomedical labeling. Zinc-based NPs, especially ZnTe and ZnSe nanoparticles, are the promising materials to fill this gap. ZnTe and ZnSe, both are important semiconductor materials with a direct band gap of 2.26 and 2.7 eV, respectively at room temperature. Synthesis of Zinc-chalcogenide nanoparticles was tried in various solvents under ultrasonic field at the multibubble sonoluminescence(MBSL) conditions. For the synthesis, we used zinc chloride, tellurium powder, selenium powder, TOP/TOPO, and HDA. Toluene was used as solvent. The particle size was controlled by changing reaction time and temperature. The prepared Zinc-chalcogenide nanoparticles are examined by XRD, ICP, UV-vis spectrophotometer, Fluorescence meter and HR-TEM.

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발표분야: 무기화학

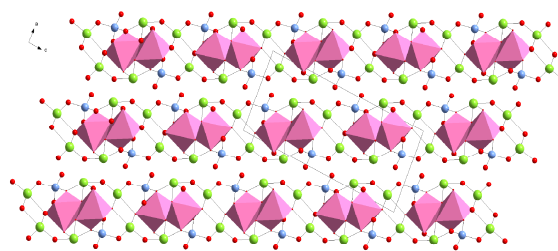
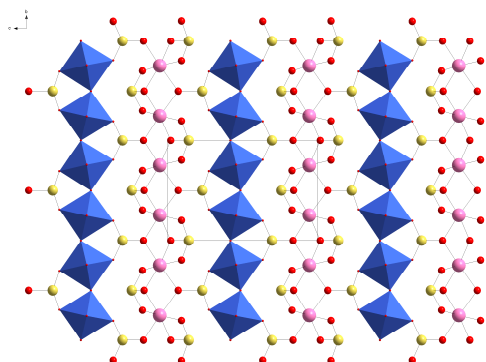
발표종류: 포스터, 발표일시: 금 10:30~12:30

## InVM<sub>2</sub>O<sub>8</sub> (M=Se and Te) : Solid-state synthesis and characterization of New Quaternary Mixed Metal Oxides.

이동우, 옥강민

중앙대 화학과

Two new quaternary mixed metal oxide materials, centrosymmetric(CS) InVTe<sub>2</sub>O<sub>8</sub> and noncentrosymmetry(NCS) InVSe<sub>2</sub>O<sub>8</sub> have been synthesized, by standard solid-state reactions using In<sub>2</sub>O<sub>3</sub>, V<sub>2</sub>O<sub>5</sub>, and TeO<sub>2</sub>(or SeO<sub>2</sub>). The centrosymmetric InVTe<sub>2</sub>O<sub>8</sub> exhibits a layered crystal structure consisting of InO<sub>6</sub> octahedra, VO<sub>4</sub> tetrahedra, and asymmetric TeO<sub>4</sub> polyhedra, and the noncentrosymmetric InVSe<sub>2</sub>O<sub>8</sub> show a 3D framework structure composed of distorted InO<sub>6</sub> octahedra, VO<sub>5</sub> square pyramids, and asymmetric SeO<sub>3</sub> polyhedra. Powder second-harmonic generation (SHG) measurements on the polar InVSe<sub>2</sub>O<sub>8</sub> using 1064 nm radiation, indicate the material has a SHG efficiency of approximately 30 × α-SiO<sub>2</sub>. Full characterization including infrared spectra, thermogravimetric analyses, UV-Vis diffuse reflectance, and dipole moment calculations are also reported.



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발표종류: 포스터, 발표일시: 금 10:30~12:30

## Synthesis of porphyrin-based microparticles with mixed building block

이준호, 이석중

고려대 화학과

Over the past decades, the self-assembly approach has become one of the most powerful techniques for synthesis of nanostructures. Particularly, porphyrins have become one of the most attractive building blocks for self-assemblies because of the enormous potential that they possess in catalysis, photochemistry, sensing, and as optical devices has made them favorite building blocks in the emerging field of molecular materials. Indeed, porphyrin building blocks have been used extensively in the construction of nano-, micro-, and macroscopic structures, including nanomaterials using  $\pi$ - $\pi$  interactions, electrostatic interactions, and metal coordination with appropriate choice of substituents. We like to introduce the synthesis and characterization of various micro crystalline particles from mixed building block such as (porphyrin)Sn(OH) with 5,15- bis(pyridyl)porphyrin or dicarboxylic acid. With various synthetic condition, they show dramatic changes on morphologies comparing with particles used only one building block.



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발표종류: 포스터, 발표일시: 금 10:30~12:30

## **Preparation and characterization of coordination driven porphyrin based crystalline microparticles**

이다희, 김선돌, 이석중

고려대 화학과

Coordination polymer has been received enormous attention due to their potential applications in catalysis, sensing, optics, separation, and recognition. Their properties are typically based on inherent characteristics of organic building blocks. In particular, Porphyrins are attractive building blocks for nanostructures because of their unique electronic, optical, catalytic, and biochemical properties. With attractive structural features such as large bulk, rigid planarity, and a highly conjugated framework that can be readily modified with a variety of functional groups, porphyrins can be assembled into supra- and super-structures in a relatively easy manner. The introduction of coordination motifs into the porphyrin building blocks offer an easy way to access well-defined coordination polymers. Furthermore, with a suitable synthetic condition these coordination polymers can be tuned in nano- or microscopic particles. In here, we like to demonstrate the synthesis and characterization of pyridine containing Zn-porphyrins base crystalline microparticles. Their morphology can be turned with a simple synthetic manipulation. We also like to show their unique electronical property.

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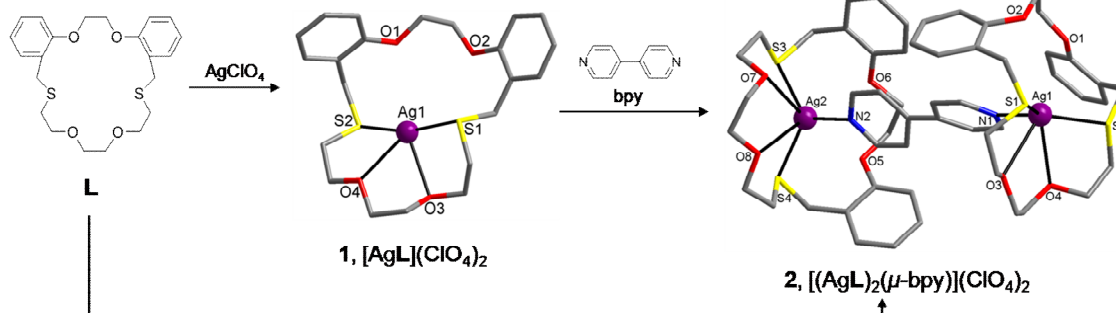
## Mono-, Di-, and Multinuclear Supramolecular Complexes of an O<sub>2</sub>S<sub>2</sub>-Macrocycle with Soft Metal Ions

주희영, 이소영, 이심성

경상대 화학과

A range of thiophilic mono-, di-, and multinuclear complexes (1-8) of the O<sub>4</sub>S<sub>2</sub>-donor macrocycle L were prepared and structurally characterized. Reaction of L with AgClO<sub>4</sub> afforded an endocyclic 1:1 complex [Ag(L)]ClO<sub>4</sub> (1) without anion binding. From the stepwise reactions of 1 followed by spacer ligands (L') such as 4,4'-bipyridine (bpy), the “dumbbell”-like complexes [(AgL)<sub>2</sub>(μ<sub>2</sub>-bpy)](ClO<sub>4</sub>)<sub>2</sub> (2) with a LAg-L'-AgL pattern were isolated (see below). The similar “dumbbell” complexes [(AgL)<sub>2</sub>(μ<sub>2</sub>-dabco)](ClO<sub>4</sub>)<sub>2</sub> (3) and [(AgL)<sub>2</sub>(μ<sub>2</sub>-bpe)](ClO<sub>4</sub>)<sub>2</sub> (4) were also isolated from the reactions of 1 with 1,4-diazabicyclo[2.2.2]octane (dabco) and 1,2-bis(pyridyl)-ethane (bpe), respectively. Mononuclear complexes with anion coordination [Hg(L)(NO<sub>3</sub>)<sub>2</sub>] (5) and [cis-Cl<sub>2</sub>Pd(L)] (6) have been prepared on the reactions of L with Hg(NO<sub>3</sub>)<sub>2</sub> and K<sub>2</sub>PdCl<sub>4</sub>, respectively. Reactions of L with AgSCN and CuBr yielded the 1D network [Ag(L)X]<sub>n</sub> (7) and [Cu<sub>2</sub>Br<sub>2</sub>(L<sub>2</sub>)]<sub>n</sub> (8), respectively.

### Route I (2-step approach)



### Route II (one-pot approach)

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## Synthesis and their photovoltaic characteristics of $\pi$ -extended Zn-porphyrins

채승현, 이영선, 이석중

고려대 화학과

In recent years, there has been considerable interest in the fabrication of photovoltaic devices using organic materials. Especially great industrial interests for 'Organic Photovoltaic Cell (OPVC)' come from their potential applications in low-cost electronic circuits such as large area and flexible displayer, active-matrix electronic-paper, and smart cards and price tags. Porphyrin derivatives are particularly attractive in OPVC because they are large and flat conjugated macrocycles whose structures can be easily tuned, and strong and tunable visible absorption properties. They have that can be controlled by simple synthetic modifications. Tetra thiophenyl Zn-Porphyrins (ZnPTs) have been synthesized by Suzuki-coupling reaction. The optical, electrochemical, photophysical, and photovoltaic properties of ZnPTs were investigated. The more extended  $\pi$ -conjugation in ZnPT shows a broad absorption with nearly visible region. Bulk heterojunction photovoltaic devices were fabricated by using the ZnPTs as donors and PCBM as an acceptor.

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## Spectroscopic studies on the interaction of native duplex DNA with bridged binuclear chiral Ru(II) complexes

프리아, \*김석규, \*\*이효선

경북대 화학과 \*영남대 화학과 \*\*경북대 자연과학대학 화학과

Abstract A pair of chiral binuclear ruthenium(II) complexes have been prepared and their binding affinities toward double stranded native DNA was assessed by means of isotropic absorption, polarized light spectroscopy including circular and linear dichroism (CD and LD), fluorescence quenching and DNA thermal denaturation techniques. The complexes produces LD signal consisting of positive and negative signal in the absorption region upon binding to DNA although these complexes exhibited red-shift and hypochromism in the absorption spectrum. These contrasting observations indicated that the binding modes of the complexes are largely deviated from classical intercalative binding. These results suggest that the groove binding nature of the complexes to DNA rather than intercalative mode of binding. The small increase of DNA melting temperature in the presence of the complex indicates predominantly DNA groove binding propensity of the complexes. Absence of "molecular light switch effect" indeed further supports non-intercalative binding mode with DNA for the new complexes. This conclusion is also supported by the comparison of the resulting data with the  $[\text{Ru}(\text{phen})_2(\text{dppz})]^{2+}$ . This study demonstrated the importance of the structure of bridging moiety in the intercalation of the Ru(II) complex.

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발표분야: 무기화학

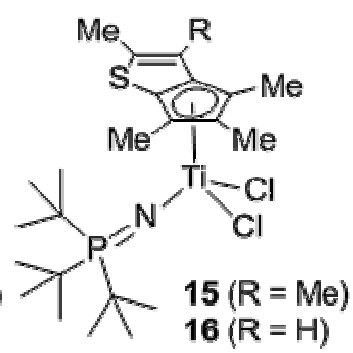
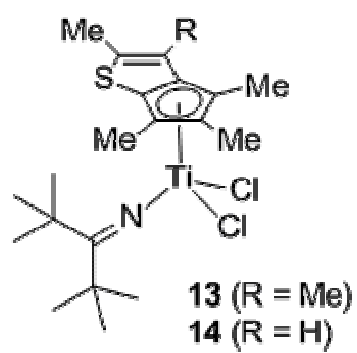
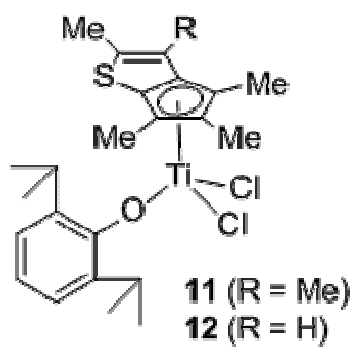
발표종류: 포스터, 발표일시: 금 10:30~12:30

## Preparation of Half-Titanocenes of Thiophene-fused Trimethylcyclopentadienyl Ligands and Their Ethylene Copolymerization Reactivity

박은석, 이분열

아주대 분자과학기술학과

Methylthiophene-fused or dimethylthiophene-fused trimethylcyclopentadienyltitanium trichloride complexes,  $(\eta^5\text{-Me}_4\text{RC}_7\text{S})\text{TiCl}_3$  ( $\text{R} = \text{Me}$  or  $\text{H}$ ), are prepared, from which a chloride ligand is replaced with 2,6-diisopropylphenoxy, di(*tert*-butyl)ketimide, or tri(*tert*-butyl)phosphinimide ligand to yield  $(\eta^5\text{-Me}_4\text{RC}_7\text{S})\text{TiXCl}_2$  (11,  $\text{R} = \text{Me}$ ,  $\text{X} = \text{iPr}_2\text{C}_6\text{H}_3\text{O}-$ ; 12,  $\text{R} = \text{H}$ ,  $\text{X} = \text{iPr}_2\text{C}_6\text{H}_3\text{O}-$ ; 13,  $\text{R} = \text{Me}$ ,  $\text{X} = \text{tBu}_2\text{C}=\text{N}-$ ; 14,  $\text{R} = \text{H}$ ,  $\text{X} = \text{tBu}_2\text{C}=\text{N}-$ ; 15,  $\text{R} = \text{Me}$ ,  $\text{X} = \text{tBu}_3\text{P}=\text{N}-$ ; 16,  $\text{R} = \text{H}$ ,  $\text{X} = \text{tBu}_3\text{P}=\text{N}-$ ). The molecular structures of 11, 14, and 16 are confirmed by X-ray crystallography. The Cp(centroid)-Ti-N angles of 11, 14, and 16 ( $119.83^\circ$ ,  $111.98^\circ$ , and  $125.34^\circ$ , respectively) are significantly larger than the corresponding angle observed for the related thiophene-fused and tetrahydroquinoline-linked cyclopentadienyl complex (1),  $[(\eta^5\text{-(Me}_4\text{C}_7\text{S)}\text{-(2-MeC}_9\text{H}_9\text{N- N)}]\text{TiMe}_2$  ( $106.6^\circ$ ). The phenoxy complexes 11 and 12 show negligible activity, while the ketimido and phosphinimido complexes 13-16 exhibit good activities ( $5\text{-}20 \times 10^6 \text{ g/molTi}\cdot\text{h}$ ) for ethylene/1-octene copolymerization. The ketimido complexes 13 and 14 are able to incorporate a high amount of 1-octene (15-16 mol%), while the phosphinimido complexes 15 and 16 are not as capable (8 mol% 1-octene) under the identical polymerization conditions. The catalytic performance of 13-16 is inferior to 1 in terms of activity and comonomer incorporation.



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발표분야: 무기화학

발표종류: 포스터, 발표일시: 금 10:30~12:30

## **[100] Directed Cu-doped h-CoO Nanorods: Elucidation of Growth Mechanism and Application to Lithium-Ion Batteries**

남기민, 박준택

KAIST 화학과

The formation mechanism of the [100] directed Cu doped h-CoO nanorods was fully elucidated by using quantum mechanics, demonstrating that Cu-doping not only changes the growth direction but also results in a significant enhancement of the stability of the h-CoO nanorods. Furthermore, the evaluation of our electrochemical performance of Cu-doped h-CoO nanorods shows their potential application to anode materials in lithium-ion batteries. High resolution TEM image and the XRD pattern clearly show Cu-doped h-CoO nanorods with an h-CoO phase. Theoretical analyses reveal that Cu-doping leads to a rearrangement of the order of surface energies among the (001), (101), (110), and (100) surfaces, thus causing the nanorods to grow along the [100] direction. The change of surface energy by doping is a crucial factor for determining the growth direction of metal-doped nanorods. This mechanism also sheds light on the formation of other wurtzite structures such as ZnO, GaN, and CdSe systems, which are known to be useful semiconductor materials. Although cubic rocksalt CoO (c-CoO) exhibits superior electrochemical features as an anode material for lithium-ion batteries, electrochemical analysis of h-CoO is unprecedented. The electrochemical properties of h-CoO nanocrystals, h-CoO nanorods, and Cu-doped h-CoO nanorods were investigated by assembling Li/h-CoO half cells. When evaluated as electrode materials for lithium-ion batteries, the as-prepared Cu-doped h-CoO nanorods show high initial Coulombic efficiency and ultrahigh capacity with excellent cycling performance for over 40 cycles, indicating their suitability as an anode material for next generation lithium-ion batteries.

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발표종류: 포스터, 발표일시: 금 10:30~12:30

## Microwave synthesis of a porous metal-organic framework, Nickel(II) dihydroxyterephthalate and its catalytic properties in oxidation of cyclohexene

심규은, \*장종산, \*\*황영규

과학기술연합대학원대 청정화학 및 생물학 \*한국화학연구원 그린화학촉매연구센터 \*\*한국화학연구원 그린화학연구단

Metal-organic frameworks(MOFs)[1,2] can be produced by an assembly of inorganic sub-units (clusters, chains, layer...) with organic linkers such as carboxylates, phosphonates, imidazolates. Recently, there is considerable interest in MOFs with high porosity and great crystallinity for use in gas storage, separation, drug release and catalysis. Among them, Nickel dehydroxyterephthalate ( $[\text{Ni}_2(\text{dhtp})(\text{H}_2\text{O})_2] \cdot 8\text{H}_2\text{O}$  (where, dhtp=2,5-dihydroxyterephthalic acid), hereafter called as Ni-DHTP), which is one of the metal-organic frameworks, have drawn a lot of attention because of high surface area, relatively high thermal stability, and a large number of coordinatively unsaturated metal sites(CUS) after removal of solvent or water molecules from the framework pores.[3]

Here, we focused on synthesis of Ni-DHTP by using microwave technique (MW). This approach aims to have better condition because microwave synthesis takes much shorter time and lower temperature than the reported synthesis via conventional heating method (CH). Also, the catalytic performances of Ni-DHTP synthesized by MW and CH methods have been studied in the oxidation of monoolefins (cyclohexene) with aqueous  $\text{H}_2\text{O}_2$  as oxidant. Ni-DHTP synthesized by MW at different synthesis temperatures and irradiation times has been found to be a good catalyst system for the oxidation of cyclohexene under milder conditions, which gave cyclohexene oxide and 2-cyclohexene-1-ol as the major products under milder oxidation conditions. In addition to Ni-DHTP, we will also report the microwave-synthesis of zirconium based MOF and sorption characteristics [4].

Reference



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2. Kitagawa, S.; Matsuda, R. *Coord. Chem. Rev.* 2007, 251, 2490.
3. Dietzel, P.D.C.; Panella, B.; Hirscher, M.; Blom, T.; Fjellvag, H. *Chem. Commun.* 2006, 959.
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발표분야: 무기화학

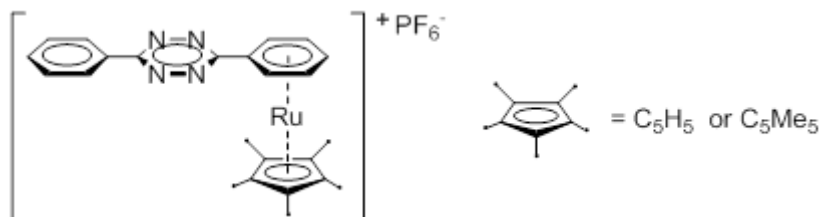
발표종류: 포스터, 발표일시: 금 10:30~12:30

## Synthesis of ( $\pi$ -3,6-diphenyl-1,2,4,5-tetrazine)Ru(Cp'=C<sub>5</sub>H<sub>5</sub>, C<sub>5</sub>Me<sub>5</sub>) Complexes

김윤희, 소혜경, \*최문근

연세대 화학과 \*연세대 이과대학 화학과

The tetrazine ring is the most electron deficient aromatic ring in the CHON chemistry, and in particular in some cases displays a  $n-\pi^*$  transition which gives rise to a particular fluorescence with especially long decay times because of the forbidden character of the transition.  $n-\pi^*$  transition whose position is dependent on the substituents. Increasing the size of the substituents makes the ring photochemically stable. Introduction of benzene ring increases the photostability and diphenyl-s-tetrazine is stable upon light irradiation. The aim of this study is synthesis of diphenyl substituted tetrazine ligands and preparation of its ruthenium complexes for studies of their photophysical properties.



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발표분야: 무기화학

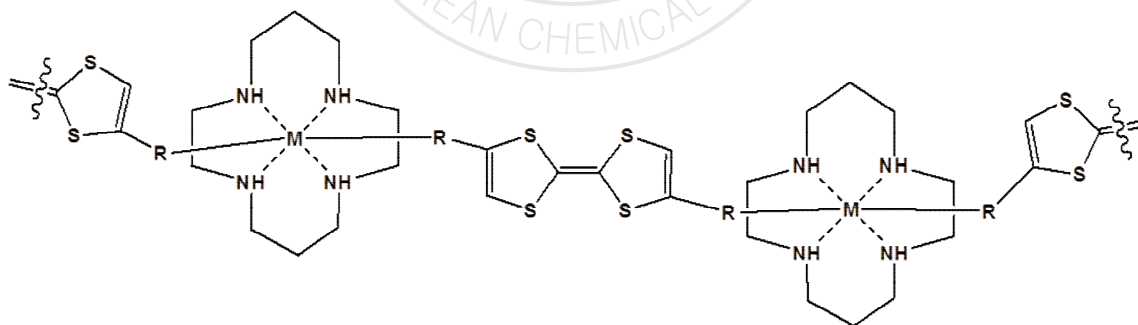
발표종류: 포스터, 발표일시: 금 10:30~12:30

## Syntheses, Characterizations of the Metal-Cyclam Complexes Containing TTF derivatives

이주은, 이홍인

경북대 화학과

TTF (tetrathiafulvalene) is a two-step electron-donor molecule, which can form charge-transfer complexes with metal ions. These complexes exhibit interesting electric and magnetic properties. In this study, we synthesize metal-TTF complexes where the metal ions are functionalized with macrocyclic ligands and the TTF molecule is functionalized with cyano groups or carboxylate groups. 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 UV.



Metal cyclam-TTF complexes의 예상 구조

M= Cu, Ni/ R= COO<sup>-</sup>/CN

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발표분야: 무기화학

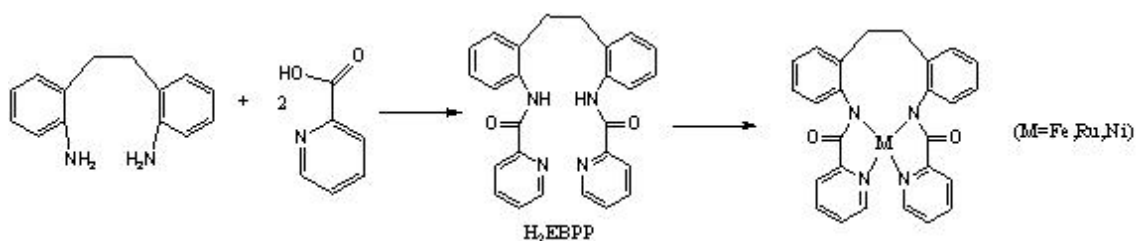
발표종류: 포스터, 발표일시: 금 10:30~12:30

## Transition Metal Complexes with *N,N'*-(ethylenedi-*p*-phenylene)bis(pyridine-2-carboxamide) Ligand : Syntheses, Characterization, Catalytic Activity

김동훈, 조장훈, 이흥인

경북대 화학과

The carboxamide group, found in the protein primary structures, is an important ligand construction unit for coordination chemistry. Metal complexes containing the carboxamide ligands have been found useful in asymmetric catalysis, molecular receptors and dendrimer synthesis. We have developed a new tetradentate ligand, H<sub>2</sub>EBPP (= *N,N'*-(ethylenedi-*p*-phenylene)bis(pyridine-2-carboxamide)), obtained from pyridyl-bearing carboxylic acids and phenyl amine via a coupling agent such as triphenylphosphite, to synthesize iron, nickel, and ruthenium complexes. In this study, we discuss the structures, physical properties, and catalytic behaviors of the complexes.



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발표분야: 무기화학

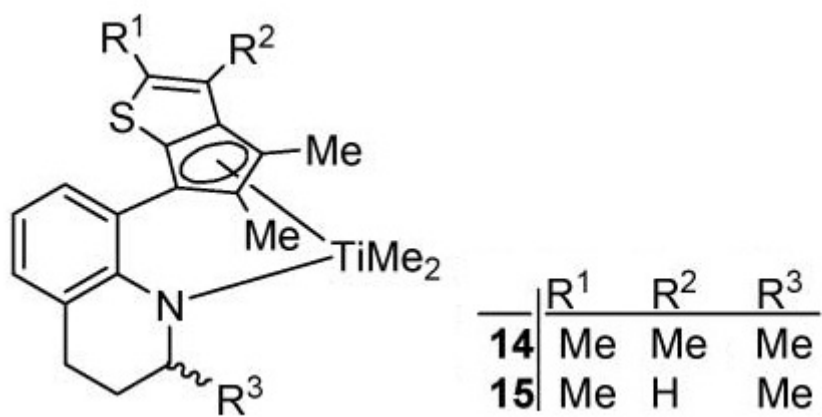
발표종류: 포스터, 발표일시: 금 10:30~12:30

## **Synthesis of half-metallocenes of thiophene-fused and tetrahydroquinoline-linked cyclopentadienyl ligands and their ethylene copolymerization reactivity.**

**박지혜, 도승현, 이분열**

아주대 분자과학기술학과

Among the homogeneous Ziegler catalysts, the dichlorotitanium (IV) complexes coordinated by both cyclopentadienyl ligands and amido ligands (half-metallocene complexes) have attracted much attention. The constrained-geometry catalyst (CGC) is a typical representative. CGC exhibits, in ethylene/ $\alpha$ -olefin copolymerizations, high activity, high  $\alpha$ -olefin incorporation, thermal stability, and high molecular weight of the obtained polymer. These performances enable its use in a commercial process. Various modifications have been carried out either by replacement of the  $\text{Me}_4\text{C}_5$ -unit with other  $\pi$ -donor ligands or by replacement of the  $\text{N}^t\text{Bu}$ -unit with other amides or phosphides. Replacement of the  $\text{Me}_2\text{Si}$ -bridge with ortho-phenylene-bridge has also been successfully achieved. This reports the preparation of half metallocene complexes constructed with the thiophene-fused cyclopentadienyls, which also showed some advantages over the conventional cyclopentadienyl analogues. Especially, the  $\text{Me}_2\text{Ti}$ -complexes 14 and 15 show excellent activities (62 and  $54 \times 10^6$  g/molTi  $\cdot$  h, respectively) in ethylene/1-octene copolymerization at 60 psig ethylene pressure even when activated with a small amount of MAO (Al/Ti = 1000).



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발표종류: 포스터, 발표일시: 금 10:30~12:30

## Synthesis of high loading Pt/solvothermal graphene using a seed mediated growth process

장병철, \*박원철

서울대 나노융합학과 \*서울대 융합과학기술대학원 나노융합학과

we could prepared high loading Pt nanoparticles on the solvothermal graphene using a combination of solvothermal method and seed mediated growth process. Graphene was prepared by reduction of ethanol using a Na metal as a reducing agent via solvothermal method. We also prepared the high loading Pt/graphene using a seed mediated growth process. The morphology of the Pt/C catalyst was characterized by using high-resolution transmission electron microscopy (HR-TEM, JEM-2010, JEOL) and field emission scanning electron microscopy (FE-SEM, S-4800, Hitachi). X-ray diffraction (XRD) patterns were obtained using a Rigaku Dmax 2500 diffractometer. The Brunauer-Emmett-Teller (BET) method was used to confirm the specific surface area via a BELSORP-mini II (BEL JAPAN) nitrogen absorption analyzer.

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발표종류: 포스터, 발표일시: 금 10:30~12:30

## **New approach to fabricate metal sulfide thin films by chemical bath deposition method using single molecule precursor**

정연구, 이진규

서울대 화학부

The semiconductor thin films fabricated by chemical bath deposition method are attracting considerable attention as it is relatively inexpensive, simple and convenient for large area deposition. We have prepared various metal sulfide thin films by a new approach of using chemical solution method, based on the mechanistic understanding of the formation of metal sulfide nanoparticles from single molecule precursors in the presence of alkylamine; nucleophilic attack of the metal-coordinated alkylamine on the most electron-deficient thiocarbonyl carbon of the alkyldithiocarbamate ligands at a low temperature initiated the decomposition to generate solid metal sulfide nanoparticles. The metal sulfide thin films have been successfully realized on the glass substrate modified with mercaptopropyltrimethoxysilane by immersing the modified glass substrate into the chemical bath of single molecule precursor (metal dialkyldithiocarbamate,  $M(DATC)_2$ ) and heating the solution in the presence of alkylamine at low temperature ( $< 150^\circ\text{C}$ ).



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발표분야: 무기화학

발표종류: 포스터, 발표일시: 금 10:30~12:30

## Synthesis and Characterization of New Copper Complex Using Chelating Ligand

조지쉐비메리, 박보근, 김창균, 정택모

한국화학연구원 화학소재연구단

Copper-based metallization has been crucial to leading-edge microelectronic industries because of its promising physical properties, such as high conductivity as well as high electromigration resistance and increased resistance to stress induced formation of voids caused by a higher melting point for copper. The chemical vapor deposition (CVD) method is one of the techniques under investigation to effectively fill high-aspect ratio holes of sub-half-micron scale. The most promising choice for a CVD precursor would be a copper compound with high vapor pressure and stability as well as low deposition temperature. We focused our study on developing Cu(II) precursors with enhanced properties. A new chelating ligand (LH) was designed and synthesized. A new copper (II) complex was synthesized by treating copper chloride and chelating ligand (LH) in toluene. The new complex has been characterized by FT-IR and elemental analysis. The properties like volatility and decomposition character of the compound has been analyzed to study the use of the new compound as a potential CVD precursor.

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발표분야: 무기화학

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## **A comparison study of catalytic properties of Gold Nanoparticles loaded mesoporous and microporous metal-organic frameworks**

**Song xiaokai**

한양대 응용화학과

A facile method was used for fabrication of gold nanoparticles (AuNPs) loaded ZIF-8\_nano, which was synthesized in methanol at room temperature with an average particle size of 50 nm. AuNPs loaded MIL-101\_micro was prepared using  $\text{HAuCl}_4 \cdot 3\text{H}_2\text{O}$  as a gold precursor and  $\text{NaBH}_4$  as a reducing reagent. Here, MIL-101\_micro was served as mesoporous template having two types of mesopores with free diameters of 2.9 and 3.4 nm, and ZIF-8\_nano was served as microporous templates having micropores with free diameter of 1.2 nm. The AuNPs loaded on both templates are highly dispersed, with a mean diameter of  $(2.3 \pm 0.7)$  nm for MIL-101\_micao and  $(3.5 \pm 0.8)$  nm for ZIF-8\_nano, respectively. To analyze the activities of Au@MIL-101 and Au@ZIF-8\_nano, the catalytic reduction of p-nitrophenol by  $\text{NaBH}_4$  was carried out as a model reaction, which has been proved to be efficient to analyze the catalytic property of metal nanostructures. The comparison study of catalytic properties of AuNPs loaded MIL-101\_micro and ZIF-8\_nano will be discussed in the presentation.

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발표분야: 무기화학

발표종류: 포스터, 발표일시: 금 10:30~12:30

## Diameter-Controlled Synthesis of Single Crystalline Topological Insulator $\text{Bi}_2\text{Se}_3$ Nanomaterials with Various Morphologies

박이슬, 이진석

숙명여대 화학과

Recently, research on  $\text{Bi}_2\text{Se}_3$  and related compounds ( $\text{Bi}_2\text{Te}_3$  and  $\text{Sb}_2\text{Te}_3$ ) has attracted much interest because they are predicted to be three-dimensional (3D) topological insulators (TIs), showing unusual phases of quantum matter with an insulating bulk gap and gapless edges or surface states. The inevitable loss and mismatch of periodic lattice structure in topological insulators could encourage atomic reconstruction and dangling bonds, these partial changes lead their surface states to be absent from the bulk properties. These distinct states in topological insulators result in different electronic properties at their insulating bulk component and the surface protected on their own boundary. Despite extensive transport experiments on bulk  $\text{Bi}_2\text{Se}_3$  since the 1970s, there has been no report of a conducting surface state, and the predicted topological features have not been addressed. Because these materials are strongly affected by the contribution of the bulk carriers, it was very hard to distinct their conductive properties originated from surface states and insulating bulk. Interestingly, it was reported that the surface conduction of topological insulator can be enhanced in the nanostructure-shaped material due to their larger surface-to-volume ratio than bulk phase. And, decreasing their size, the contribution of the bulk carriers can be suppressed and the contribution of surface states, which could affect the electrical and optical properties, is enhanced. With this background in mind, we tried to synthesize single crystalline  $\text{Bi}_2\text{Se}_3$  nanomaterials using chemical vapor deposition (CVD) method, including their characterization. From different reaction conditions such as temperature, pressure and gas flow rates, they are synthesized in the form of various morphologies and diameter through a gold-catalyzed vapor-liquid-solid (VLS) growth process.

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발표분야: 무기화학

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## Controlled Growth of Bent Silicon Nanowires Through Change of Growth Kinetics

박이슬, 정다희, 이진석

숙명여대 화학과

As the development of nanowire fabrication advances, there is considerable interest in extending 1D nanowire growth to more complex structures of higher dimensionality such as may be used to form interconnects for electronic circuits with the controlled size and direction. The development of a technology for programmatically directing the position of nanowire branch-points takes a first step toward the general creation of higher dimensional structures, including axial nanowire and branched nanowire heterostructures. Previously, branched nanowire structures have been demonstrated using both chemical synthesis and vapor-liquid-solid (VLS) synthesis methods. In principle, the VLS synthesis method should provide a means for directing nanowire growth from arbitrary branch locations. To date, research in 3D branched wire structures has been carried out using random deposition of catalyst nanoparticles resulting in randomly branched nanowires. In this research, we demonstrate that the abrupt change of growth kinetics can affect the bending growth in the end of silicon nanowires. And, we propose advanced CVD method to control the bending position and growth direction without the additional seeding process of catalysts. In order to control the degree of bending, we varied several experimental parameters such as flow rate, source injection time and cooling state. Using this technique, various structures including multiple bendings and several generations of nanowires were expected to be fabricated.

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발표분야: 무기화학

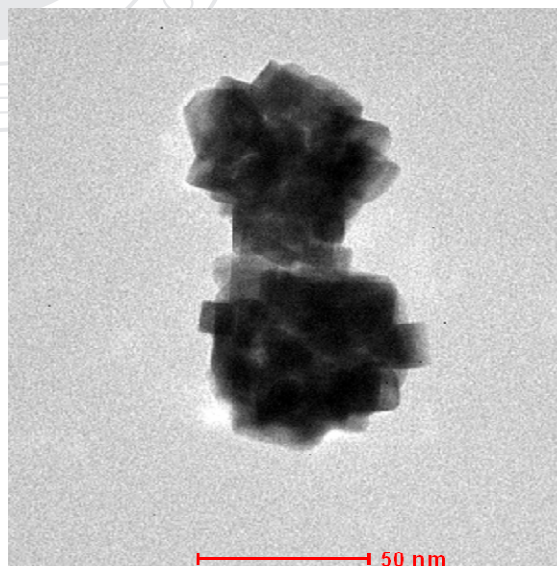
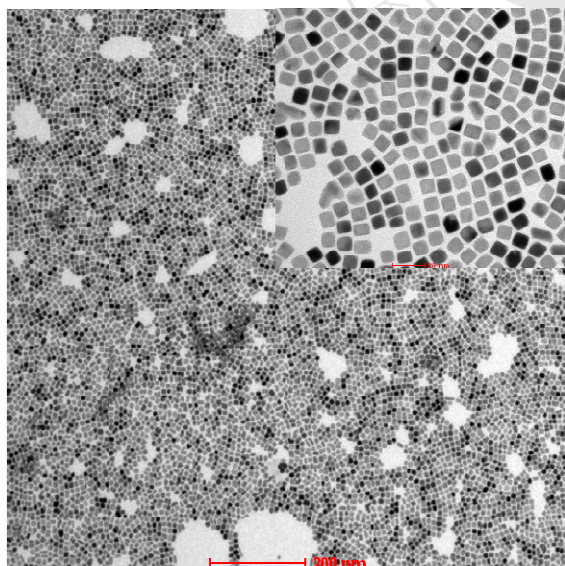
발표종류: 포스터, 발표일시: 금 10:30~12:30

## Formation of Gas-induced Pt Nanocubes and Nanolegos

이강열, \*이광렬

고려대 기초과학연구원 \*고려대 화학과

We report a solution-phase synthesis of Pt nanocubes and nanolegos by using the CO(g) and Ar(g) gas. The nanocubes were synthesized by controlled in the presence of only CO gas, while nanolegos were obtained via the secondary growth of polyhedral particles on the vertices of the unripe Pt nanocrystals in the presence of Ar and CO gas. The prepared Pt nanostructures were characterized by transmission electron microscopy, scanning electron microscopy, powder X-ray diffraction, and electron dispersive spectroscopy.



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발표분야: 무기화학

발표종류: 포스터, 발표일시: 금 10:30~12:30

## Synthesis, Characterization, and Application of Ultrasmall (~4nm) and Monodisperse $\text{Fe}_x\text{Co}_{1-x}$ -Graphite Shell Nanocrystals

최인애, 서원석

서강대 화학과

We have prepared ultrasmall and monodisperse  $\text{Fe}_x\text{Co}_{1-x}$ -graphitic carbon shell (FeCo/GC,  $x = 0.12, 0.36, 0.42, 0.50, 0.56, 0.62$ ) nanocrystals with an average diameter of 4 nm in a mesopores silica support by using a simple CVD method. The prepared nanocrystals were characterized by X-ray diffraction (XRD), TEM, SQUID, and MRI. The Fe/Co ratios of the FeCo/GC nanocrystals can be tuned by changing the Fe/Co ratios of the metal precursors. As the Fe contents of the FeCo/GC nanocrystals were increased, these crystal structures were changed from mixed structures of body-centred-cubic (bcc) FeCo and face-centred-cubic (fcc) Co to pure bcc FeCo.  $\text{Fe}_{0.56}\text{Co}_{0.44}$ /GC nanocrystals showed the highest saturation magnetization of 200 e.m.u.  $\text{g}^{-1}$  at 300 K and the highest  $r_1$  and  $r_2$  relaxivities as magnetic resonance imaging (MRI) contrast agents. The FeCo/GC nanocrystals are expected to show multifunctional biomedical applications including MRI, drug delivery, and near-infrared agents.

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발표코드: III-INOR.P-91

발표분야: 무기화학

발표종류: 포스터, 발표일시: 금 10:30~12:30

## **The control of 3-dimensional 10nm scale pattern of secondary sputtering lithography by varying poly styrene pattern.**

전환진, 정희태

KAIST 생명화학공학과

The development of large-area nano-patterning with high resolution, high aspect ratio and simple process scheme/cost is a challenging work for realizing their potential applications in opto-electronics and nano-biotechnology such as nanoelectronics, optics, optical sensing, light-emitting devices and bio-sensing devices. Several approaches towards nanostructure fabrication have been exploited without resorting to expensive tools such as those used in deep-UV projection lithography and electron-beam lithography. We have reported powerful patterning method named secondary sputtering lithography in the past year. This novel patterning technology enables to fabricate the high resolution of complex nanoscale patterns with simple process. The idea arises from the angular distribution of target particles by ion-beam bombardment, which use the ultra-thin nano structure in consistent with side shape of polymer patterns by attaching target materials to the polymer surfaces during accelerated ion-assisted bombardment. Here, we demonstrate that the high resolution of complex nanoscale patterns can be controlled by simple PS treatment process. The PS pattern can be controlled by simple pattern transfer step and reactive ion etching.

일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: III-INOR.P-92

발표분야: 무기화학

발표종류: 포스터, 발표일시: 금 10:30~12:30

## Synthesis of New Sr-Ti Bimetallic Complex for Strontium Titanate (SrTiO<sub>3</sub>) Material

김효숙, 박보근, 김창균, 정택모

한국화학연구원 화학소재연구단

In recent years, thin films of SrTiO<sub>3</sub>(STO) have been intensively investigated for the application to capacitor dielectrics for future dynamic random access memory(DRAM). Strontium Titanate (SrTiO<sub>3</sub>) has been greatly focused on because of its variety of outstanding physical properties: (i) an insulator-metal transition and superconductivity at low temperatures by electron doping, (ii) the formation of a two-dimensional electron gas at interfaces between SrTiO<sub>3</sub> and other oxides, (iii) blue light emission in Ar-irradiated, electron-doped, and O-deficient SrTiO<sub>3</sub>, and (iv) ferroelectricity without any intentional doping. Therefore, we will present the design, synthesis of Sr-Ti bimetallic complex and characterization by NMR, FT-IR, elemental analysis, and TGA.



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발표코드: III-INOR.P-93

발표분야: 무기화학

발표종류: 포스터, 발표일시: 금 10:30~12:30

## Novel Chlorotitanium Complexes Containing Tetrazole

이준승, 고민정, 김세란, 강이영, 오창화

전남대 화학과

A series of new half-sandwich titanocene  $[(\eta^5\text{-C}_5\text{H}_5)\text{TiLCl}_2]$  (1) and non-organometallic titanium complexes  $[\text{TiLCl}_3(\text{THF})]$  (2) and  $[\text{TiL}_2\text{Cl}_2]$  (3) containing 5-(2-hydroxyphenyl)tetrazole (LH) were synthesized in high yield by an HCl elimination reaction and fully characterized by various spectroscopic methods. Molecular structures of compounds 1 – 3 were determined by X-ray crystallography. In all complexes, ligand L acted as a monoanionic bidentate ligand and the hydrogen bonding between the oxygen of the tetrahydrofuran and hydrogen of the tetrazolyl unit was observed. Although 1 – 3 lack typical initiating groups such as alkoxides or amides, they are effective catalysts for the ring opening polymerization of lactide (LA) as shown by the linearity of molecular weight vs  $[\text{LA}]/[\text{Ti}]$  ratio plot as well as narrow polydispersity index values.

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장소: 제주ICC

발표코드: III-INOR.P-94

발표분야: 무기화학

발표종류: 포스터, 발표일시: 금 10:30~12:30

## Highly Stable and Magnetically Recyclable Mesoporous Silica Spheres Embedded with FeCo-Graphite Shell Nanocrystals for Supported Catalysis

LIYAN, \*김연진, \*\*박강현, \*서원석

서강대 바이오융합 \*서강대 화학과 \*\*부산대 화학과

We have synthesized highly stable and magnetically recyclable mesoporous silica spheres embedded with FeCo-graphitic carbon shell nanocrystals (MSS@FeCo/GC) by a simple one-step CVD method. Solid core-mesoporous shell silica spheres with an average diameter of ~400 nm were used as supports not only for the synthesis of the FeCo/GC nanocrystals but also for catalysts after the synthesis of the MSS@FeCo/GC. The FeCo/GC nanocrystals in the mesoporous silica spheres exhibit superparamagnetism with ultra-high saturation magnetization up to 215 emu/metal g at room temperature. The FeCo/GC nanocrystals are chemically stable against acid etching and oxidation, which enable the MSS@FeCo/GC to be stable in acidic catalytic conditions and even support acid catalyst, phosphomolybdic acid (PMA). We have shown that PMA supported on MSS@FeCo/GC works as an excellent recyclable solid reagent system.

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장소: 제주ICC

발표코드: III-INOR.P-95

발표분야: 무기화학

발표종류: 포스터, 발표일시: 금 10:30~12:30

## **Fabrication of multi-segment line pattern by photo- and soft lithography**

이지선, 정희태

KAIST 생명화학공학과

One-dimensional nanostructures, such as an array of nanowires, exhibit distinct electronic, optical, chemical and thermal properties due to their large surface area and possible quantum confinement effects. The multiple functionalization of heterojunction nanowires which consist of alternatively arranged metal segments are very attractive approach to find out novel functionality and phenomena, offering promise for a range of application, including nanoscale electronics and sensor technology. In this research, we report novel method to fabricate multiple segments line pattern through soft-lithography combined with conventional photolithography technique. Firstly, we generate pre-line patterned substrate which has alternative line array two different materials in micro-scale by using photolithograph, Ion-milling and lift-off process. Then, we create polymer line pattern in nano-scale using CFL in perpendicular direction upon the substrate which is made by photolithography, after etch uncovered part of metal substrate, we can finally obtain multi-segmented line-pattern array. Our approach offers very effective way to produce highly arranged linepattern with high throughput and facile manner. We expected this kind of linepattern can be functionalized differently in each segment so that we can use it as a sensor, transistor or waveguide of electronic, biological or optical devices.

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장소: 제주ICC

발표코드: III-INOR.P-96

발표분야: 무기화학

발표종류: 포스터, 발표일시: 금 10:30~12:30

## Synthesis and Characterization of novel 1,1-Difunctional Germafluorene and their polymerization for the Detection of Nitramines.

엄성용, 조현, 김희철, 손홍래

조선대 화학과

New functionalized germafluorenes have been synthesized and their optical and electronic characterizations were investigated. The compounds were synthesized by a stepwise reactions of the bis(dibromobenzene) with germanium tetrachloride in THF at room temperature. The germafluorenes were characterized by  $^1\text{H-NMR}$ ,  $^{13}\text{C-NMR}$ , UV-vis absorption, and photoluminescence spectroscopy. The optical absorption spectra showed an absorption edge at 285 nm, while a strong UV-vis photoluminescence at 350 nm is observed. 1,1-difunctional germafluorenes was served as a chemical sensor. Detection of nitroaromatics, nitramines, and nitrate esters were investigated by measuring the quenching photoluminescence of 1,1-difunctionalgermafluorene.

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장소: 제주ICC

발표코드: III-INOR.P-97

발표분야: 무기화학

발표종류: 포스터, 발표일시: 금 10:30~12:30

## **Bio-functionalization of Siloles and Silafluorenes for the Detection of Biomolecules**

조현, 엄성용, 이보연, 손홍래

조선대 화학과

The synthesis of the highly fluorescent siloles and silafluorenes derivatized with biotin was investigated for searching a possible application as biosensor. 1- methyl-1-hydro-2,3,4,5-tetraphenylsilole and 1-methyl-1-hydro-silafluorene were derivatized with allylamines to give amine functionalized silole and silafluorene via hydrosilylation. Amine-functionalized silole and silafluorene were further derivatized with biotin to give biotin-functionalized silole and silafluorene. All silole and silafluorene derivatives were characterized with  $^1\text{H}$ - and  $^{13}\text{C}$ -NMR spectroscopy. Optical characterization were carried out with UV-Vis absorption and fluorescence spectroscopy. These biotin-functionalized molecules were used for the detection of biomolecules such as avidin and streptavidin through the quenching of photoluminescence. Detection mechanism and further details will be discussed.

일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: III-INOR.P-98

발표분야: 무기화학

발표종류: 포스터, 발표일시: 금 10:30~12:30

## Development of Synthetic Routes for Silicon Quantum Dots and Their Optical Characterization.

김희철, 엄성용, 황민우, 손홍래

조선대 화학과

Silicon quantum dots (QDs) embedded in a dielectric matrix have immense potential in devices such as next-generation photovoltaic solar cells, light-emitting diodes, thin-film transistors as well as other applications. This is why nanocrystalline Si-based nanophase materials have a distinct advantage over bulk Si which exhibits an indirect bandgap, which in turn requires phonon interactions when absorbing or emitting photons. While bulk Si has very weak luminescence due to its indirect band gap, nanosized silicon quantum dots (Si QDs) possess more efficient luminescence. Silicon QDs are also nontoxic and cheap when compared to well-investigated II-VI semiconductors that contain cadmium. In addition, Si QDs are expected to integrate easily into well-established industrial silicon processes. The synthesis of Si QDs, where n-butyl-capped Si QDs possessed an average diameter of approximately 6.5 nm was achieved by using silicon tetrachloride and sodium/benzophenone in ethylene glycol dimethyl ether. The optical band gaps and reflective indices of Si QDs were investigated. Si QDs prepared displayed very weak photoluminescence due to the defects in the silicon crystal net work. To overcome this issues, new synthetic routes for the Si QDs has been investigated. The solvents for the crystal growth and the reaction temperature have been varied to investigate the photoluminescence efficiency of silicon quantum dots. Their refractive indices were monitored to determine the optical band gaps. Polyperchlorosilanes are synthesized as a precursor for the synthesis of silicon nanoparticles.

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장소: 제주ICC

발표코드: III-INOR.P-99

발표분야: 무기화학

발표종류: 포스터, 발표일시: 금 10:30~12:30

## Synthesis, Characterization, and Application of Silafluorene-Phenyleneethynylene Alternating Copolymers

이보연, 조보민, 조현, 손홍래

조선대 화학과

Silafluorene-phenyleneethynylene alternating copolymers were synthesized from the reaction of dihydrosilafluorene and 1,4-bis(tetradecyloxy)-2,5-diiodobenzene via palladium-catalyzed cross-coupling. These copolymers were characterized by  $^1\text{H}$ - and  $^{13}\text{C}$ -NMR spectroscopy. Photoluminescence of these copolymers were measured by fluorescence spectrometer. Quantum efficiencies of these polymers from the quantum yield of corresponding silafluorene monomer unit were investigated. Detection of nitramines, nitroaromatics, and nitrate esters were investigated by using these copolymers through the quenching of photoluminescence. Quenching behavior obtained from the detection of nitroaromatic compounds will be discussed as a chemical thin films. The rapid fluorescence response (quenching) of the spin-cast films of to nitro-containing compounds qualifies these materials as promising TNT chemosensory materials.

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장소: 제주ICC

발표코드: III-INOR.P-100

발표분야: 무기화학

발표종류: 포스터, 발표일시: 금 10:30~12:30

## Electronic and Optical Characterization of silafluorenes Their application for the Detection of RDX

황민우, 조보민, 김희철, 손홍래

조선대 화학과

1,1-Dimethylsilafluorenes and 1,1-diphenylsilafluorenes were synthesized and their electronic and photonic behaviors have been investigated. The synthesized compounds were characterized by  $^1\text{H}$  and  $^{13}\text{C}$  NMR spectroscopy. Absorption and emission spectra for these compounds were obtained by using UV-Visible and fluorescence spectroscopy in solution. Their emission behaviors and quantum yield for these compounds were investigated both in the solid and colloid state. Our results indicated that both compounds were used as the chemosensor to detect nitroamines, (1,3,5-trinitroperhydro-1,3,5-triazine, RDX), nitroaromatics (1,3,5-trinitrotoluene, TNT), and nitrate esters (PETN). The detection efficiency results shown that both compounds were served as the chemosensors and indicated that 1,1-diphenylsilafluorenes gave higher detection efficiency than 1,1-Dimethylsilafluorenes. Other silafluorene derivatives were synthesized and their photonic behaviour were investigated. Further details will be presented.



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장소: 제주ICC

발표코드: III-INOR.P-101

발표분야: 무기화학

발표종류: 포스터, 발표일시: 금 10:30~12:30

## Two dimensional metal-organic framework based on Zn(II), 1,3,5-benzene tricarboxylic acid and p-diimidazolate ligand

박지혜, 유대원, 구봉호, 홍창섭

고려대 화학과

We have synthesized two-dimensional metal-organic framework,  $[Zn(p\text{-dim})(BTC)] \cdot H_2O \cdot DMA$  ( $p\text{-dim}$  = 1,4-di(1H-imidazol-5-yl)benzene,  $BTC$  = 1,3,5-benzene tricarboxylic acid) under the solvothermal reaction of  $p\text{-dim}$ ,  $BTC$  and  $ZnBr_2$  in mixed solvent of DMF, DMA and  $H_2O$ . We have revealed that the 2D-framework has  $Zn(II)$  ion coordinated by carboxylates( $-CO_2$ ) originating from  $BTC$ , and two nitrogen atoms of  $p\text{-dim}$  using x-ray crystallography. This 2D framework is stable due to interaction between 6-membered ring and 5-membered ring of  $p\text{-dim}$  and H-bonding between amide of  $p\text{-dim}$  and carboxylate of  $BTC$ . The further structural features and physical properties of the MOF will be discussed.

일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: III-INOR.P-102

발표분야: 무기화학

발표종류: 포스터, 발표일시: 금 10:30~12:30

## Synthesis of cyanide-Bridged One-Dimensional Fe(III)-Mn(III) Complexes Based on a New *mer* - Positioned Fe(III) Cyanide Precursor : Synthesis, Crystal Structures, and Magnetic Characterizations

손아랍, 윤정희, 유대원, 구봉호, 홍창섭

고려대 화학과

A new *mer*-[LFe<sup>III</sup>(CN)<sub>3</sub>]<sup>-</sup> precursor with chelating ligands of 8-(6-bromopyridine-2-carboxamido)quinoline anion (6-Brpcq), was prepared. Three Fe(III)Mn(III) bimetallic compounds, [Fe(6-Brpcq)(CN)<sub>3</sub>][Mn(5-Xsalen)]·xsol, [salen = N,N'-ethylenebis(salicylideneiminato)dianion; X=H(1), Cl(2), Br(3)] were prepared by assembling the precursor and the respective Mn Schiff bases. Compounds 1-3 show linear chain structures in which *trans*-positioned cyanides of the Fe precursor bridge neighbouring Mn atoms. Detailed structural and magnetic studies will be given in the presentation.

일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: III-INOR.P-103

발표분야: 무기화학

발표종류: 포스터, 발표일시: 금 10:30~12:30

## Structural Transformations in the Cu MOF Toward Zn and Tb MOFs : Crystal structures and Gas Sorption Properties

이우람, 홍창섭

고려대 화학과

We have synthesized a copper compound with a three dimensional network structure using a solvothermal reaction of  $H_3TPO$  ( $H_3TPO = 4,4',4''$ -phosphoryltribenzoic acid) in DMF, water and methanol mixed solvent. We demonstrate the structure, sorption properties and structure transformations of a new coordination polymer having the formula  $[Cu(TPO)](DMF)_2(H_2O)_{1.5}$  (1), solvothermal reaction of copper nitrate hydrate and  $H_3TPO$  gave clear green crystals (Yield >90%). The void volume of network 1 is  $2588.3 \text{ \AA}^3$  per unit cell, which is 44.2% of the total crystal volume. When 1 was immersed in zinc nitrate and terbium nitrate in DMF for 60 h at  $100^\circ\text{C}$ , both complexes were exchanged by  $Zn(II)$  and  $Tb(III)$  ions as confirmed by single crystal X-ray diffraction and luminescence properties. Structures, sorption and luminescent properties of the title compounds will be presented in detail.

일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: III-INOR.P-104

발표분야: 무기화학

발표종류: 포스터, 발표일시: 금 10:30~12:30

## Three-dimensional bimetallic complex built with the copper(II) metalloligand and Mn(III) Schiff base exhibiting magnetic property and sorption

유대원, 홍창섭

고려대 화학과

A three dimensional porous complex,  $[\text{Cu}(\text{Tt})_2\{\text{Mn}(\text{salen})\}_2](\text{ClO}_4)_2 \cdot 4\text{H}_2\text{O}$  [Tt=tris(1,2,4-triazolyl)borate], was prepared by a slow evaporation in mixed solvent of  $\text{H}_2\text{O}$  and MeCN. This complex is composed of the metalloligand  $[\text{Cu}(\text{Tt})_2]$  with six exodentate sites and Mn(III) Schiff base. The Mn(III) is coordinated by two axial N atoms from metalloligand and the isolated  $[\text{ClO}_4]^-$  anions are present in the structure to maintain charge balance. Although the anions exist, the pore size is sufficient to adsorb guest molecules. We will present the detailed structure, sorption and magnetic properties in the presentation.

일시: 2011년 4월 28~29일(목~금) 2일간

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발표코드: III-INOR.P-105

발표분야: 무기화학

발표종류: 포스터, 발표일시: 금 10:30~12:30

## Photoluminescent Silicon Nanoparticles Containing Camptothecin for Drug Delivery Applications

류정관, 손홍래

조선대 화학과

Photoluminescent silicon nanoparticles chemically bounded 20(S)-Camptothecin (CPT) were used for noble drug delivery materials and prepared from the porous silicon by using ultra sonic fracture. Luminescent porous silicons were obtained by an electrochemical etching of n-type single crystalline silicon wafer. Luminescent porous silicon was air-oxidized and its surface was derivatized with 20(S)-Camptothecin. Camptothecin-derivatized porous silicon was fractured by ultrasono-method to give a luminescent silicon nanoparticles. The size of these particle were in the range from few nm to few microns. Optical characteristics of CPT-derivatized silicon nanoparticles were investigated. The release of CPT from silicon nanoparticles were studied. Detailed experimental results will be discussed.

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장소: 제주ICC

발표코드: III-INOR.P-106

발표분야: 무기화학

발표종류: 포스터, 발표일시: 금 10:30~12:30

## Gold nanowires synthesized using polymer

박민균, \*최세범, \*\*유현웅

연세대 화공생명공학과 \*충북대 공업화학과 \*\*한국표준과학연구원 미래융합기술부

골드 나노구조는 높은 전도성을 가지고 있어서 나노스케일 전자 장비와 센서 등에 많이 사용된다. 골드 나노구조를 합성하는 방법으로는 template assisted synthesis, assembly of nanoparticles, surfactant mediated growth 등이 있는데 폴리머를 사용한 방법은 앞선 방법에 비해 높은 aspect ratios 를 가지며 매우 얇은 골드 나노구조를 합성 할 수 있다. 본 연구에서는 폴리머를 사용한 합성에서 은 나노입자 대신 다른 물질을 사용했을 때 골드 나노와이어 합성여부와 구조를 살펴보고 다른 입자를 사용하지 않을 때의 골드 나노와이어의 수율을 높이는 방법에 대해 살펴보겠다. 골드 나노구조에 따른 변화는 주사전자현미경(SEM), 자외선 분광기(UV), 투과전자현미경(TEM)을 이용하여 확인하였다.

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장소: 제주ICC

발표코드: III-INOR.P-107

발표분야: 무기화학

발표종류: 포스터, 발표일시: 금 10:30~12:30

## **Fabrication of Gradient Optical Filter Containing Anisotropic Bragg Nanostructure**

조보민, 이보연, 황민우, 손홍래

조선대 화학과

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

일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: III-INOR.P-108

발표분야: 무기화학

발표종류: 포스터, 발표일시: 금 10:30~12:30

## Thermal decomposition mechanism of single-molecule precursors forming metal oxide nanoparticles.

김태근, \*조준상, 정연구, 이진규

서울대 화학부 \*서울대 화학부/화학과

Metal oxide 나노입자 합성에 많이 사용되는 대표적 organometallic precursor 인 metal oleate  $[M(C_{18}H_{33}O_2)_2]$ 가 alkylamine 의 존재 하에서 thermal decomposition 되는 반응 mechanism 에 대한 연구를 진행하였다. Cadmium, zinc, manganese, 그리고 iron 과 같은 다양한 금속 전구체의 thermal decomposition 과정에서 alkylamine 의 역할에 대한 mechanism 을 관찰하였다. Metal oleate 가 alkylamine 과 thermal decomposition 될 때 형성되는 side product 와 metal oxide nanoparticle 은 NMR, GC-MS, XRD, TEM 으로 분석하여, metal 전구체에 배위 결합한 amine 이 가장 전자가 결핍된 oleate 의 oxycarbonyl carbon 에 nucleophilic attack 을 하면서 분해반응이 시작되어 물, 유기물 side product, solid metal oxide nanoparticles 이 형성되는 공통된 결과가 확인되었다. 이러한 결과로부터 organometallic precursor 의 일반적인 분해 mechanism 과 alkylamine 의 역할을 규명하였다.



일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: III-INOR.P-109

발표분야: 무기화학

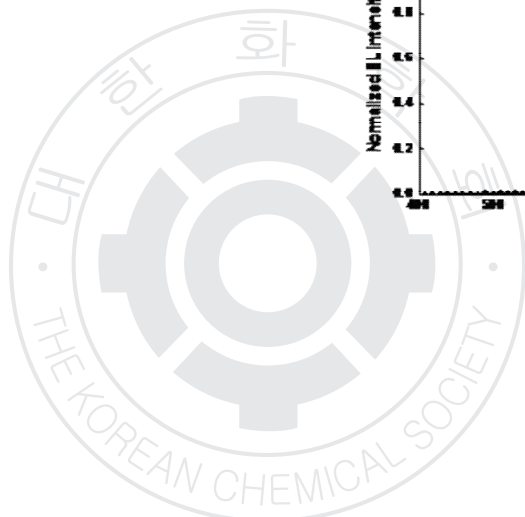
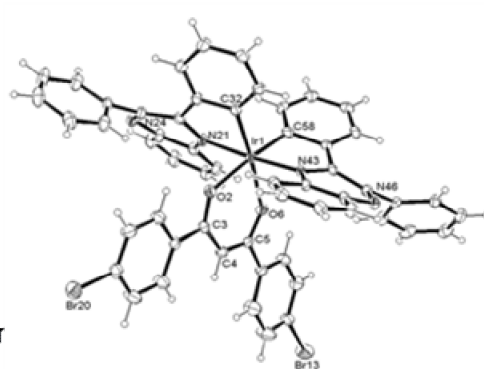
발표종류: 포스터, 발표일시: 금 10:30~12:30

## Ir(III) Complex with Conjugated 1,3-Bis(p-bromophenyl)-1,3-propanedione for Red Organic Light-Emitting Diodes

김인찬, \*송영광, 윤성재, \*김대영, \*\*김영인

부산대 화학과 \*부산대 첨단정보 및 디스플레이소재협동과정 \*\*부산대 화학교육과

The deep-red emitting iridium(III) complexes with extended  $\pi$ -conjugation system were designed, synthesized and characterized for organic light-emitting diodes (OLEDs);  $(N^{\wedge}C)_2Ir(O^{\wedge}O)$ , where  $N^{\wedge}C$ =2-phenylbenzothiazole, 2,3-diphenylquinoxaline and  $O^{\wedge}O$ =1,3-bis(*p*-bromophenyl)-1,3-propanedione;  $(pbt)_2Ir(dbacac)$  (1),  $(dpq)_2Ir(dbacac)$  (2).



일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: III-INOR.P-110

발표분야: 무기화학

발표종류: 포스터, 발표일시: 금 10:30~12:30

## Synthesis of Novel Ta precursors using ALD/CVD

신수정

고려대 화학과

Tantalum nitride ( $\text{TaN}_x$ ) films have been an attractive candidate as a diffusion barrier, gate electrode for CMOS (complementary metal oxide semiconductor), and electrodes for capacitors used in memory devices. Also Tantalum carbo-nitride ( $\text{TaCN}$ ) films has been studied as a gate electrode in the next generation nano-CMOS technology for its low resistivity, proper work function and high reliability. We synthesized novel Ta precursors for TaN and TaCN Thin Film Deposition using ALD/CVD process. All compounds have been characterized by means of NMR spectrometry, FT-IR, elemental analysis, and TGA.

일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: III-INOR.P-111

발표분야: 무기화학

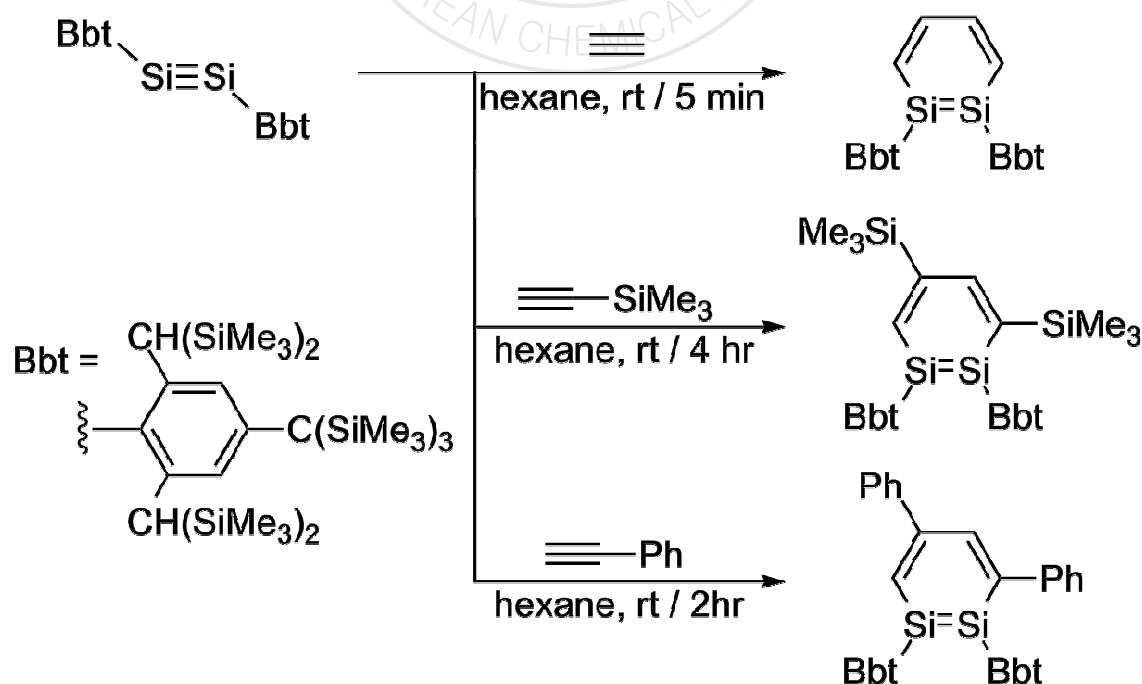
발표종류: 포스터, 발표일시: 금 10:30~12:30

## Disilabenzenes from the Reactions of a 1,2-Diaryldisilyne with Alkynes

한준수, \*T. Sasamori, \*Y. Mizuhata, \*N. Tokitoh

KIST 나노재료센터 \*Kyoto University, Japan

Since the first isolation of a silaaromatic compound (a stable 2-silanaphthalene) in 1997, the chemistry of silaaromatic compounds has attracted much interest in recent decades. On the other hand, recent achievements in the synthesis of disilyne, compounds having a Si-Si triple bond, gave us the opportunity to explore the reactivity of disilynes. A series of 1,2-disilabenzenes were synthesized from the reaction of a 1,2-diaryldisilyne with alkynes. Crystal structure of a 1,2-disilabenzene shows that the central ring skeleton has an almost planar structure. Here we discuss the further evidences for the aromatic nature of the 1,2-disilabenzene in view of both experimental and theoretical results.



일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: III-INOR.P-112

발표분야: 무기화학

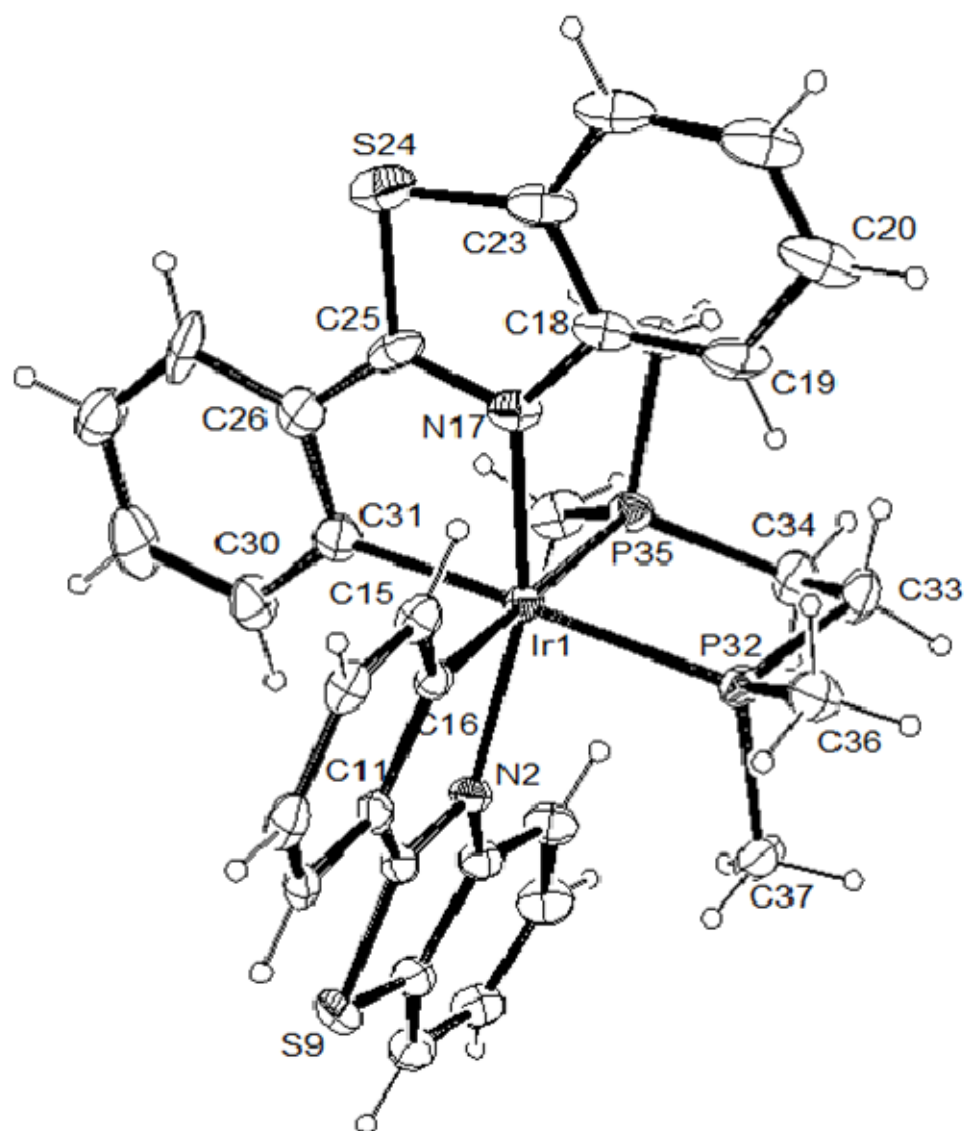
발표종류: 포스터, 발표일시: 금 10:30~12:30

## Phosphorescent Heteroleptic Ir(III) Complexes with 2-(2-Hydroxyphenyl)benzothiazole

윤성재, \*송영광, 김인찬, \*\*황인혜, \*\*김영인

부산대 화학과 \*부산대 첨단정보 및 디스플레이소재협동과정 \*\*부산대 화학교육과

New heteroleptic iridium(III) complexes,  $(N^{\wedge}C)_2Ir(P^{\wedge}P)$ , containing two  $(N^{\wedge}C)$  ligands and one  $(P^{\wedge}P)$  diphosphine ligand were prepared :  $(pbt)_2Ir(dmpe)$  (1),  $(pbt)_2Ir(dppe)$  (2) and  $(dpq)_2Ir(dppe)$  (3), where  $pbt=2$ -phenylbenzothiazole,  $dpq=2,3$ -diphenylquinoxaline,  $dmpe=1,2$ -bis(dimethylphosphino)ethane and  $dppe=1,2$ -bis(diphenylphosphino)ethane. The structural and photophysical and electrochemical properties were investigated. The complexes exhibited the photoluminescence peaks at 503 ~ 586 nm and quantum yields of 34 ~ 52% in solution. The structure of (1) showed that the iridium(III) centers adopted a distorted octahedral coordination geometry with cis C-C and trans N-N arrangements. The OLED was fabricated using complex (3) and the performance was examined.



일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: III-INOR.P-113

발표분야: 무기화학

발표종류: 포스터, 발표일시: 금 10:30~12:30

## Easy and versatile functionalization of lithium niobate crystal toward the application of SAW device

김보람, 강원석, \*고광락, 김재호

아주대 분자과학기술학과 \*부산대 나노과학기술대학

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 3-aminopropyltriethoxysilane-modified lithium niobate surface is largely due to the formation of a siloxy-niobate ( $-\text{Si}-\text{O}-\text{Nb}-$ ) bond via a condensation reaction between ethoxysilane ( $-\text{Si}-\text{O}-\text{C}-$ ) and niobate hydroxide ( $-\text{NbOH}$ ). The extremely hydrophobic and stable SAM on lithium niobate could have useful applications in surface acoustic waves (SAW) device.

일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: III-INOR.P-114

발표분야: 무기화학

발표종류: 포스터, 발표일시: 금 10:30~12:30

## Synthesis of Cu-In-Se using the single-source precursor

한정민

한국화학연구원 화학소재연구단

SSPs prepared via this new route have successfully been used in a spray assisted chemical vapor deposition (CVD) process to deposit polycrystalline thin films, and for preparing ternary nanocrystallites. The Cu-In-Se ternary system has attracted much attention with applications in the area of solar cells, non-linear optics and optical communications. In this study, we have demonstrated for the first time the synthesis of ternary Cu-In-Se using the single-source precursor (SSP).



일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: III-INOR.P-115

발표분야: 무기화학

발표종류: 포스터, 발표일시: 금 10:30~12:30

## Kinetic Mechanism of Quaternary Quantum Dot $\text{Cd}_x\text{SexZn}_{1-x}\text{S}_{1-x}$ in II-VI Semiconductor Nanocrystal Synthesis

조준상, \*정연구, \*이진규

서울대 화학부/화학과 \*서울대 화학부

II-VI 족 quaternary quantum dot ( $\text{Cd}_x\text{SexZn}_{1-x}\text{S}_{1-x}$ ) formation kinetic 을 UV-Vis absorption spectroscopy, photoluminescence (PL) spectroscopy, nuclear magnetic resonance (NMR) spectroscopy, inductively coupled plasma atomic emission spectroscopy (ICP-AES), transmission electron microscopy (TEM)을 이용하여 연구하였다. Quaternary quantum dot 을 형성하는 각각의 metal precursor 와 chalcogenide precursor 의 반응성의 차이에 기초한 이들의 농도 변화를 통하여 quantum dot 의 emission wavelength 를 조절할 수 있었다. 그리고 oleylamine 존재하 metal precursor 의 thermal decomposition 속도 변화로 인한 quantum dot 의 composition 이 변하였고, 그에 따른 emission wavelength 조절도 가능하였다. 우리는 II-VI 족 quaternary quantum dot ( $\text{Cd}_x\text{SexZn}_{1-x}\text{S}_{1-x}$ ) formation kinetic 를 바탕으로 metal 과 chalcogenide 의 reactivity 를 control 하여 II-VI 족 quaternary quantum dot 의 formation mechanism 을 제시하였고 quaternary quantum dot 의 composition 을 규명하였다.

일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: III-INOR.P-116

발표분야: 무기화학

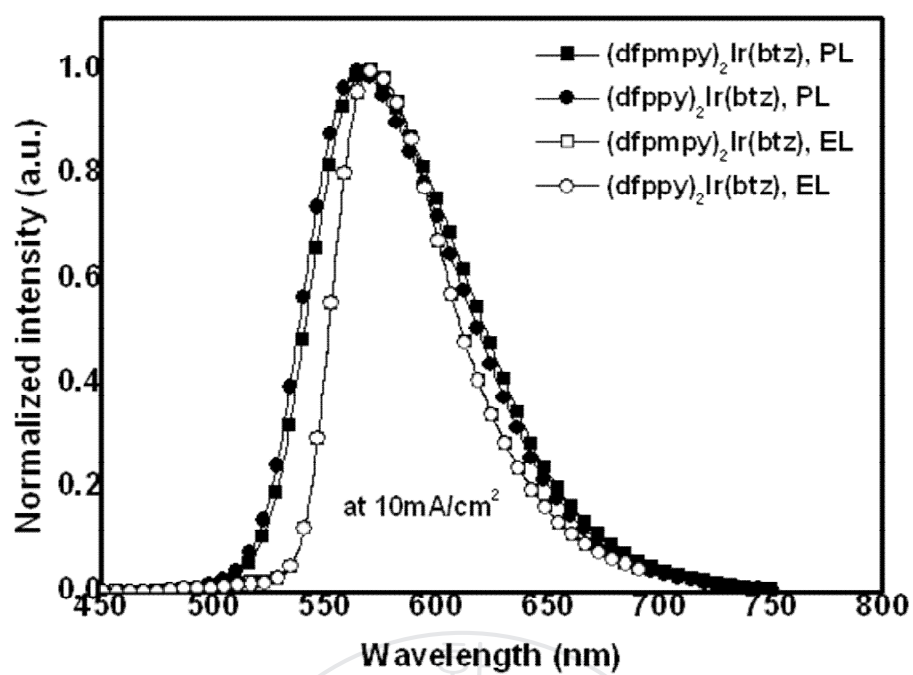
발표종류: 포스터, 발표일시: 금 10:30~12:30

## Phosphorescent Heteroleptic Ir(III) Complexes with 2-(2-Hydroxyphenyl)benzothiazole

송영광, \*윤성재, \*김인찬, 김대영, \*\*김영인

부산대 첨단정보 및 디스플레이소재협동과정 \*부산대 화학과 \*\*부산대 화학교육과

We have designed and synthesized heteroleptic Ir(III) complexes,  $(C^N)_2Ir(N^O)$ , where  $C^N$  = 2-phenylbenzothiazole, 2-(2,4-difluorophenyl)pyridine (dfppy), 2-(2,4-difluorophenyl)-5-methylpyridine (dfpmpy) and  $N^O$  = 2-(2-hydroxyphenyl)benzothiazole;  $(pbt)_2Ir(btz)$  (1),  $(dfppy)_2Ir(btz)$  (2),  $(dfpmpy)_2Ir(btz)$  (3). The complexes exhibited the photoluminescence peak at 564 ~ 580 nm and quantum yields of 8 ~ 31 % in solution. The electroluminescent properties of complex (2) and (3) were studied to show orange emission, CIE coordinates of (0.53, 0.46) with a maximum external quantum efficiency of 4.24% and luminance efficiency of  $9.90 \text{ cd A}^{-1}$ .



일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: III-INOR.P-117

발표분야: 무기화학

발표종류: 포스터, 발표일시: 금 10:30~12:30

## Selective encapsulation of meta-stable sulfur by porous coordination network

최완욱, \*Nazrul Islam, Masaki Kawano

포항공과대 첨단재료과학부 \*POSTECH, Korea

Porous coordination networks have been extensively studied because of their fascinating features like guest encapsulation, sorption/storage/separation of gases ( $H_2$ ,  $CO_2$ ,  $CH_4$ , etc.), drug delivery using uniform pore size and high surface area. However, the usages of such porous materials are mainly confined to deal with stable molecules. In nature, elemental sulfur mostly exists as stable  $S_8$  ring with a small amount of unstable  $S_7$ ,  $S_6$  and other forms as a mixture. Here we first report that a porous network can selectively encapsulate meta-stable sulfur into a pore in the gas phase. We will report a crystal structure of the sulfur-encapsulated network determined by ab initio powder X-ray diffraction analysis and the characterization by EA, TG-DSC, and spectroscopy.

일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: III-INOR.P-118

발표분야: 무기화학

발표종류: 포스터, 발표일시: 금 10:30~12:30

## Design of redox-active porous coordination network

구진영, Yakiyama Yumi, \*Yasushi Morita, Masaki Kawano

포항공과대 첨단재료과학부 \*Department of Chemistry, Graduate School of Science, Osaka  
University

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-diazaphenylene (DAP). Furthermore, we synthesized several network structures composed of DAP and various metal sources. It is noteworthy that negative charge delocalization occurs in the deprotonated central azaphenalenyl skeleton in these networks which will afford unique physical properties. This is the first example of a highly redox-active coordination network. Here, we will report X-ray analysis of DAP-based networks and their physical properties in detail.

일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: III-INOR.P-119

발표분야: 무기화학

발표종류: 포스터, 발표일시: 금 10:30~12:30

## Polydiacetylene coated silica NPs and their fluorescence property

경산, 이윤식

서울대 화학생물공학부

Polydiacetylene (PDA) has been used in many fields because of its interesting properties; the polymerization ability from exposure of ultraviolet rays without any initiators or catalysts and the chromic nature by external stimuli e.g. heat, stress and molecular recognitions. In here, we immobilized PDA on to quantum dot (QD) embedded silica nanoparticles (PDA-QD2) and analyzed its optical properties. The prepared PDA-QD2 exhibits a blue color without fluorescence by PDA. After inducing stress, PDA-QD2 changed its color from blue to red with fluorescence of PDA. And we recognized the QD fluorescence over the PDA background that could be used as multiplexing detection. Moreover, our PDA immobilization methods are successfully applied to various size of QD2.

일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: III-INOR.P-120

발표분야: 무기화학

발표종류: 포스터, 발표일시: 금 10:30~12:30

## **Hydrogen Adsorption and Crystal Field within Nano-pores of Zeolites - Investigated by the In-situ Neutron Powder Diffraction Experiments at HANARO**

이희주, 최용남, \*윤경병

한국원자력연구소 중성자과학연구부 \*서강대 화학과

Neutron scattering is a useful and powerful tool for the investigation of positions and motions of materials in the atomic level. Especially, because of their unique sensitivity to hydrogen (deuterium), it can be used to probe the behaviors of hydrogen atoms or molecules in the matters. In this study, in-situ neutron diffraction experiments were carried out to investigate the adsorption mechanism of two kinds of zeolites, a cation rich system (ETS-10 and Cr-exchanged ETS-10) and the opposite system (ZSM5, Silicalite), by measuring the diffraction patterns and the adsorption capacity ( $c(P,T)$ ), simultaneously ( $T : 30 \sim 300$  K,  $P : 0 \sim 100$  bar). The experimental results and discussions on the correlation between the adsorption capacity and the crystal field from the cations which induces the hydrogen polarizability will be presented.

일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: III-INOR.P-121

발표분야: 무기화학

발표종류: 포스터, 발표일시: 금 10:30~12:30

## Syntheses and Characterization of Tin(IV) Porphyrin-based Multichromophoric Arrays

박수영, 이민정, 노수민, 김희준

금오공과대 응용화학과

Development of photovoltaic materials is of much current interest. It requires careful selection of photo and redox-active components arranged in an appropriate manner. Multichromophoric arrays, able to capture visible light photons and electron transfer, are essential targets to construct artificial-photosynthetic devices for photovoltaic and optoelectronic applications. Porphyrins are attractive molecular components for the design of artificial photosynthetic systems and applications in molecular photoelectronic materials and devices because of their unique structures and rich photoelectronic properties. We have been interested in the design of well-defined donor-acceptor systems based on tin(IV) porphyrins and other chromophores such as fullerene, dithienylethene, viologen, subphthalocyanines and boron dipyrromethenes via axial coordination. We here present the preparation and characterization of tin(IV) porphyrin-based multichromophoric arrays including subphthalocyanine and boron dipyrromethenes.



일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: III-INOR.P-122

발표분야: 무기화학

발표종류: 포스터, 발표일시: 금 10:30~12:30

## Recognition of Alkylammonium Cations by Tin(IV) Porphyrins

이미희, 김희준

금오공과대 응용화학과

Tin(IV) porphyrins have drawn recent attention in the architectures of supramolecular porphyrin arrays because of their useful coordination properties conferred by the highly charged main group metal center. In particular, 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. We here present the recognition of alkylammonium cations by dihydroxotin(IV) pyridylporphyrins using cooperative interaction of axial ligand and peripheral functional group.

일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: III-INOR.P-123

발표분야: 무기화학

발표종류: 포스터, 발표일시: 금 10:30~12:30

## Supramolecular Assembly of Porphyrin-Viologen Dyads with Cucurbit[7]uril and Their Photophysical Properties

김민경, 김빛나라, 김희준

금오공과대 응용화학과

Multicomponent donor-acceptor systems and their photo-induced energy or electron transfer processes have been received great attention with the goals of understanding the primary processes in natural photosynthesis and of designing photochemical molecular devices for energy conversion. Porphyrins are popularly employed as suitable photoactive components in multicomponent systems. On the other hand, viologen (4,4-bipyridinium dication, V<sup>2+</sup>) is a common electron acceptor in studies of electron transfer reactions. The inclusion complexes of viologen dication in larger cucurbit[n]uril homologues (CB[n], n = 7 and 8), are thermodynamically and kinetically stable. Thus, we have been interested in supramolecular manipulation of photoinduced electron transfer processes in porphyrin-viologen dyads with cucurbit[7]uril. Photophysical and photochemical studies of these types of multi-component molecular and supramolecular systems would be very useful for understanding the fundamental photoinduced electron transfer processes in photosynthesis, and consequently for creating the light driven system. Here we present the syntheses of porphyrin-viologen dyads, its inclusion behaviors in CB[7], and their photophysical properties.

일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: III-INOR.P-124

발표분야: 무기화학

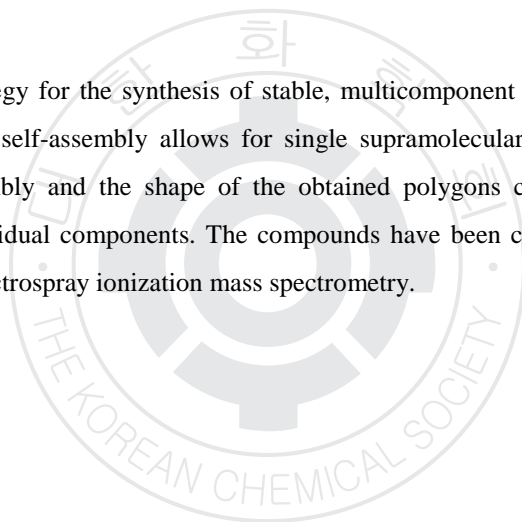
발표종류: 포스터, 발표일시: 금 10:30~12:30

## Simple Shape control of Polygons

이준승, 고민정, 강이영, 오창화, 김세란

전남대 화학과

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. The compounds have been characterized by multinuclear NMR spectroscopy and electrospray ionization mass spectrometry.



일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: III-INOR.P-125

발표분야: 무기화학

발표종류: 포스터, 발표일시: 금 10:30~12:30

## **Novel Pd catalysts for the Copolymerization of functionalized nonpolar norbornene with bulk olefin**

이용준, 안명용, 이익모

인하대 화학과

Polynorbornene has been a good candidate for the optical devices working in the short wavelength but brittleness prevented this material from further applications. Copolymerization of functional polar norbornenes with nonpolar norbornenes would be a possible method for the improvement of properties of norbornenes. In our search for the active catalytic systems for the polymerization of functional norbornenes, we found that Pd complexes with  $\beta$ -diketiminates were quite soluble in common organic solvents but highly stable in water. Emulsion copolymerization of functional norbornenes with nonpolar norbornenes has been achieved in the presence of Pd complexes with  $\beta$ -diketiminates and the effects of various reaction parameters have been investigated. In this presentation, preparation and copolymerization behaviors of an efficient catalytic system will be discussed.

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장소: 제주ICC

발표코드: I-PHYS.P-1

발표분야: 물리화학

발표종류: 포스터, 발표일시: 목 10:30~12:30

## **Role of water on $\alpha$ -helix stabilization of peptide bearing all-hydrocarbon crosslink**

홍주연, 함시현

숙명여대 화학과

Recent studies have shown that the introduction of all-hydrocarbon crosslink into  $\alpha$ -helical peptide can provide increased  $\alpha$ -helical contents, thermal and chemical stabilities, protease stability, binding ability for their target receptors, and cellular uptake. Accordingly, we performed the molecular dynamics simulations and 3D-RISM calculation to understand the high thermal stability of  $\alpha$ -helix conformations by using the cell-penetrating poly-arginine peptide. These theoretical approaches explain the important role of water on enhanced helicity of  $\alpha$ -helical peptide bearing hydrocarbon crosslink by using the protein energetics, solvation free energy, and radial distribution function analyses.

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장소: 제주ICC

발표코드: I-PHYS.P-2

발표분야: 물리화학

발표종류: 포스터, 발표일시: 목 10:30~12:30

## Understanding the effect of stereochemistry of the staples in the $\alpha$ -helix stabilization: Replica exchange molecular dynamics simulation study

홍주연, 함시현

숙명여대 화학과

Recent work has shown that  $\alpha$ -helix peptides bearing all-hydrocarbon crosslink (staple) can greatly increase their  $\alpha$ -helix propensity, leading to an improvement in pharmaceutical properties such as proteolytic stability, receptor affinity, and cell permeability. Especially, S,S-configuration stapled system with i, i+4 crosslink provided a significantly increased stabilizing effect and efficient cellular uptake on the stapled peptides over other combinations of stereochemistry. Herein, the molecular details of structural and thermodynamic behaviors for stapled peptides will be presented with different stereochemistry by using the replica exchange molecular dynamics (REMD) simulation results.

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장소: 제주ICC

발표코드: I-PHYS.P-3

발표분야: 물리화학

발표종류: 포스터, 발표일시: 목 10:30~12:30

## **Configurational entropy of protein: A combined approach based on molecular simulation and integral-equation theory of liquids**

정성호, 함시현

숙명여대 화학과

We report the recent development of a theoretical method to calculate the protein configurational entropy in explicit solvent from statistical properties of the solvent-averaged protein potential energy surface. This method can be implemented via a combined approach based on molecular simulation and integral-equation theory of liquids. Our method does not assume Gaussian distribution of protein configurations, and can be applied to unfolded or misfolded states of protein in which an average protein structure is not well defined. An illustrative application is made to misfolded state of 42-residue amyloid beta protein in water.

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장소: 제주ICC

발표코드: I-PHYS.P-4

발표분야: 물리화학

발표종류: 포스터, 발표일시: 목 10:30~12:30

## Understanding Conformational Transitions of Alanine Dipeptide Using Self-Guided Molecular Dynamics Simulation

박미래, \*Bernard R. Brooks, 함시현

숙명여대 화학과 \*Laboratory of Computational Biology, NHLBI, NIH

Although conventional molecular dynamics (MD) simulation is a useful tool for searching conformational transition pathways, it has limitation of time scale. To overcome the problem, a number of methods have been proposed. Among presented methods, self-guided molecular dynamics (SGMD) simulation enhances conformational search efficiency through acceleration of low frequency motions in a molecular system. In this study, we have investigated conformational transitions of alanine dipeptide using SGMD simulation in explicit water to compare efficiency between conventional MD and SGMD methods.



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장소: 제주ICC

발표코드: I-PHYS.P-5

발표분야: 물리화학

발표종류: 포스터, 발표일시: 목 10:30~12:30

## **Stapling Effects on the Stabilization of 3<sub>10</sub>-Helix by Molecular Dynamics Simulations in Explicit Water**

박미래, 함시현

숙명여대 화학과

Recent studies have shown that the incorporation of a 'staple', a hydrocarbon crosslink, to  $\alpha$ -helical peptide backbone can greatly increase helical content, binding affinity for target receptor, and in vivo half-life leading to an improvement in pharmaceutical properties. Herein, we report the stapling effects of 3<sub>10</sub>-helix by all-atom molecular dynamics simulations in explicit water. We will focus on structural behavior such as 3<sub>10</sub>-helical contents comparing staples encompassing one turn (i, i+3 staple) with different stereochemistry.

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장소: 제주ICC

발표코드: I-PHYS.P-6

발표분야: 물리화학

발표종류: 포스터, 발표일시: 목 10:30~12:30

## Exploring the Dissociation Process of Ab42 by Molecular Dynamics in Explicit Water

박미래, 함시현

숙명여대 화학과

Aggregates of 42-residue b-amyloid (Ab42) protein are considered as a primary agent of Alzheimer's disease (AD). Recently, increasing evidence suggests that Ab oligomers are the direct effectors of synaptic and cognitive dysfunctions. In addition, Ab dimers impair synaptic plasticity and memory. Although a numerous research has been focused on structures and aggregations Ab oligomers, the mechanisms and driving forces for Ab aggregation are not yet known. Here, we report the dissociation process of Ab42 dimer using extensive all-atom MD simulations in explicit water environment.

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장소: 제주ICC

발표코드: I-PHYS.P-7

발표분야: 물리화학

발표종류: 포스터, 발표일시: 목 10:30~12:30

## **A-to-E Backbone Mutation Effects on the Amyloid Fibril Fragment $A\beta_{(16-20)}$ by Quantum Mechanical Calculations**

김다솜, 함시현

숙명여대 화학과

Amyloid fibril structures are stabilized by intermolecular hydrogen bond in  $\beta$ -sheets. We replaced the amide NH with an ester O (amide-to-ester mutation) of leucine and phenylalanine on the second  $\beta$ -strand in  $A\beta_{16-20}$  dimer to evaluate backbone-backbone hydrogen bond effect. We performed quantum mechanical calculation to investigate the amide-to-ester mutation effect on the geometric and energetic properties of antiparallel and parallel  $A\beta_{16-20}$  dimers at the HF/3-21G\* and MPWB1K/3-21G\*//HF/3-21G\* level of theory.

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장소: 제주ICC

발표코드: I-PHYS.P-8

발표분야: 물리화학

발표종류: 포스터, 발표일시: 목 10:30~12:30

## Quantum mechanical study on the amyloid fibril fragment A $\beta$ (16-20)

김다솜, 함시현

숙명여대 화학과

Alzheimer's disease has characteristic of aggregation of amyloid- $\beta$  peptides. Hydrogen bonds between peptide backbones and hydrophobic interactions are known to be important in stabilizing  $\beta$ -sheets conformation in amyloid- $\beta$  aggregates. Here, we report the results of the structural and energetic properties of antiparallel and parallel A $\beta_{16-20}$  dimers by using quantum chemical calculation at the HF/3-21G\* and MPWB1K/3-21G\*//HF/3-21G\* level.

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장소: 제주ICC

발표코드: I-PHYS.P-9

발표분야: 물리화학

발표종류: 포스터, 발표일시: 목 10:30~12:30

## Computational studies on the hydrolysis of methyl triphosphate (MTP)

김윤진, 함시현

숙명여대 화학과

In living cells, adenosine triphosphate (ATP) is considered as the universal energy-transfer molecule. Despite of the extensive experimental and theoretical studies to elucidate where the energy is stored in ATP, no clear conclusion has been reported. Therefore, we performed theoretical calculations on the hydrolysis reactions of methyl triphosphate (MTP) as a model system for ATP by combining DFT calculations and 3D-RISM theory. The equilibrium structures of MTP with four different charged states (-4, -3, -2, -1) and the products of hydrolysis reaction were explored both in a gas phase and in an aqueous phase to figure out hydrolysis energy, Gibb's free energy, entropy, and enthalpy of the reactions. We here report the thermodynamics properties of MTP hydrolysis reactions and the contribution of hydrolysis reactions in energy storage and transduction.

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장소: 제주ICC

발표코드: I -PHYS.P-10

발표분야: 물리화학

발표종류: 포스터, 발표일시: 목 10:30~12:30

## Why A $\beta$ 42 aggregates faster than A $\beta$ 40?

원주희, \*정성호, 함시현

숙명여대 화학과 \*서울대 화학부

Physiological 40-residue and 42-residue amyloid-beta protein (A $\beta$ 40 and A $\beta$ 42) are major components of amyloid plaques associated with Alzheimer's disease. Although they differ in only two amino acid residues at the C-terminal end, A $\beta$ 42 is much more prone to aggregate and more toxic than A $\beta$ 40. To investigate the molecular origin on the differences in the aggregation propensities between those two proteins, we have performed comparative study of A $\beta$ 40 and A $\beta$ 42 monomers in explicit water by using all-atom molecular dynamics simulations in water. We here report the simulation results based on the trajectory analyses on A $\beta$ 40 and A $\beta$ 42 in water focusing on the effects caused by two extra residues in A $\beta$ 42.

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장소: 제주ICC

발표코드: I-PHYS.P-11

발표분야: 물리화학

발표종류: 포스터, 발표일시: 목 10:30~12:30

## **DFT study on the amide-to-ester backbone mutation effect of N-methylacetamide (NMA) clusters**

손아영, 함시현

숙명여대 화학과

One of the major components constructing protein 3D-structure is the backbone-backbone hydrogen bonds (H-bonds). The importance of backbone H-bonds can be evaluated by the backbone mutation substituting amide NH to ester O. This substitution of a main chain, so-called amide-to-ester mutation has been used to investigate the role of the polypeptide backbone-backbone H-bond interactions. In this regard, we performed theoretical calculations on n-mer (1~3) of a model peptide, N-methylacetamide (NMA), and its mutant methyl acetate (MA) to quantitatively explore the backbone H-bonding effect in NMA clusters. We also compared optimized geometries, energetics, charge distributions, and interaction energies of each model system to evaluate H-bonding effect by using density functional theory at the B3LYP/6-311++G\*\* level.

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장소: 제주ICC

발표코드: I -PHYS.P-12

발표분야: 물리화학

발표종류: 포스터, 발표일시: 목 10:30~12:30

## **Understanding the Enzyme Properties of Subtilisin Carlsberg in Aqueous and Nonaqueous Media Using Molecular Dynamics Simulations**

조선희, 함시현

숙명여대 화학과

Enzymes have been used to catalyze various transformations of biological and industrial significance in nonaqueous media. According to the experimental studies, changing the level of solvent polarity causes the variations of the enzyme activity. To understand solvation effects of the enzyme activity in nonaqueous media, we have simulated serine protease Subtilisin Carlsberg as a model system. Herein, we present the results from molecular dynamics simulations of Subtilisin Carlsberg in three different media (chloroform, methanol, and water) to understand protein dynamics depends on media polarity.



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발표코드: I-PHYS.P-13

발표분야: 물리화학

발표종류: 포스터, 발표일시: 목 10:30~12:30

## Solvothermal synthesis of CdSe/ZnS nanoparticles using ionic liquids as capping ligands and Graphene Hybrids

송윤미, \*명윤, \*장동명, \*장소영, \*박정희, \*\*차은희

고려대 소재화학과 태양에너지소재 \*고려대 소재화학과 \*\*호서대 화학

Ionic liquids are room-temperature molten salts, composed of organic mostly of organic ions that may undergo almost unlimited structural variation. We studied the effects of ionic liquids as capping ligand and/or solvent, on the morphology and phase of the CdSe/ZnS nanoparticles. Colloidal CdSe/ZnS nanoparticles were synthesized using a series of imidazolium ionic liquids; 1-R-3-methylimidazolium bis(trifluoromethylsulfonyl)imide ([RMIM][TFSI]), where R = ethyl ([EMIM]), butyl ([BMIM]), hexyl ([HMIM]), octyl ([OMIM]). In particular, the morphology evolves from dots to rods upon the longer alkyl chains of imidazolium cation. We also synthesized the nanoparticles using a mixture of trihexyltetradecylphosphonium bis(trifluoromethylsulfonyl)imide ([P6,6,6,14][TFSI]) and octadecene (ODE). The CdSe/ZnS nanoparticles have a smaller size than that synthesized using imidazolium, and with a controlled phase from zinc-blende to wurtzite by increasing the volume ratio of [P6,6,6,14][TFSI]. CdSe/ZnS nanoparticles and graphene hybrids were synthesized using ionic liquid as a linker and showing the higher photocurrent for the nanorods than the nanodots.

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장소: 제주ICC

발표코드: I-PHYS.P-14

발표분야: 물리화학

발표종류: 포스터, 발표일시: 목 10:30~12:30

## Optical properties of Nb<sub>2</sub>O<sub>5</sub>@ CdS<sub>x</sub>Se<sub>1-x</sub> Nanocables using vapor transport method

강준하, 박정희

고려대 소재화학과

Ternary alloy Nb<sub>2</sub>O<sub>5</sub>@ CdS<sub>x</sub>Se<sub>1-x</sub> nanocables were successfully grown through a one-step thermal evaporation route using Au catalyst and Nb<sub>2</sub>O<sub>5</sub> NWs substrate. The nanostructures obtained are uniform in diameter, and have smooth surfaces. High-resolution transmission electron microscopy, energy dispersive x-ray spectra and x-ray diffraction showed that both the nanowires and the nanocables shell are high-quality single-crystalline structures, and their compositions can be determined pure CdS, diverse Sulfur ratio give a concrete example CdS<sub>0.85</sub>Se<sub>0.15</sub>, CdS<sub>0.6</sub>Se<sub>0.4</sub>, CdS<sub>0.2</sub>Se<sub>0.8</sub> etc. ,and pure CdSe respectively. The photoluminescence and UV-vis measurements showed very strong band-edge emission for samples, which further demonstrates the single-crystal nature of the as-obtained CdS<sub>x</sub>Se<sub>1-x</sub> alloys. This finding may be extended for fabrication their composition tunable 1D ternary alloy nanostructures.

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발표코드: I-PHYS.P-15

발표분야: 물리화학

발표종류: 포스터, 발표일시: 목 10:30~12:30

## Charge-Selective Raman Scattering by “Ag nanoparticles On Carbon and Nitrogen doping Silicon Nanowires” Substrates

백선영, 박정희

고려대 소재화학과

Monolayers of metal nanoparticles (NPs) have gained significant interest as surface plasmon resonance (SPR) sensors, surface-enhanced Raman scattering (SERS) substrates, and other plasmonic devices. An interesting feature in NPs monolayers is the nanoparticle charge, which can be exploited in self-assembly, as well as selective adsorption of ions on NPs. Monolayers of silver nanoparticles (Ag NPs) were synthesized on carbon doping and nitrogen doping silicon nanowires arrays using Successive Ionic Layered Absorption and Reaction (SILAR) method, were shown to exhibit charge-selective surface-enhanced Raman scattering and fluorescence quenching. Interestingly, the doping type, whether C- or N, is found to have a strong impact on the particle coalescence during electroless reduction. Because SERS has strong dependence on nanostructure, dissimilar Ag NPs structures obtained by electroless reduction on C- and N-doping Si NWs arrays cannot help elucidate the role of nanoparticles charge on SERS.

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발표코드: I -PHYS.P-16

발표분야: 물리화학

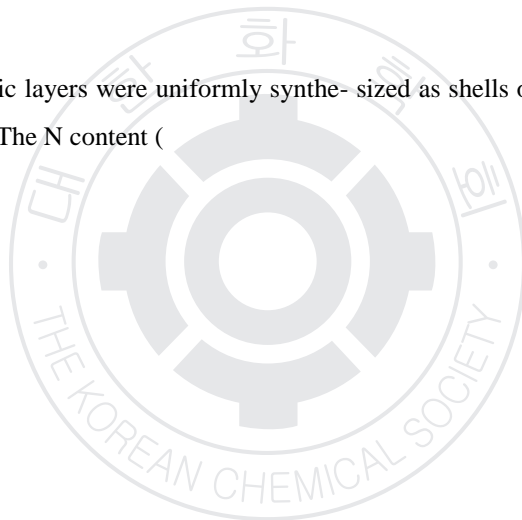
발표종류: 포스터, 발표일시: 목 10:30~12:30

## Selective Nitrogen-Doping Structure of Nanosize Graphitic Layers

조용재, 김한성, 백선영, 명윤, 정찬수, 김창현, 박정희, \*강홍석

고려대 소재화학과 \*전주대 나노신소재공학과

Nitrogen (N)-doped graphitic layers were uniformly synthesized as shells on pregrown Si nanowires by chemical vapor deposition. The N content (



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발표분야: 물리화학

발표종류: 포스터, 발표일시: 목 10:30~12:30

## **Synthesis of Mn doped GaAs, GaP nanowires and their magnetic properties.**

임형순, \*박정희

고려대 미세소자공학협동 \*고려대 소재화학과

GaAs, GaP nanowires were synthesized and Mn doped by the vapor transport method. They consisted of single-crystalline zinc blende GaAs nanocrystals (avg. diameter = 100 nm) grown along the [111] direction. The Mn doping increases the lattice constant, most significantly. X-ray absorption spectroscopy and X-ray magnetic circular dichroism confirmed that the Mn<sup>2+</sup> ions substitute into the tetrahedrally coordinated Ga sites. The magnetization measurement revealed that all of these nanowires exhibited roomtemperature ferromagnetic behavior.

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장소: 제주ICC

발표코드: I-PHYS.P-18

발표분야: 물리화학

발표종류: 포스터, 발표일시: 목 10:30~12:30

## **TiO<sub>2</sub>/Ge, ZnO/Ge and Si/Ge core/shell Nanocable Arrays and their Enhancement of Photocurrent Properties.**

임영록, 조용재, 명윤, 김한성, 김창현, 박정희

고려대 소재화학과

Vertically-aligned TiO<sub>2</sub>-, ZnO-, and Si-Ge core-shell nanocable arrays were synthesized by vapor phase deposition of Ge layers on the pre-grown nanowires at a large area of substrates. The thickness of the Ge outerlayers is controlled in the range 20 ~ 50nm. The morphology and structure of the products were analyzed by scanning electron microscopy (SEM), Energy dispersive X-ray spectroscopy (EDX), high-resolution transmission electron microscopy (HRTEM), X-ray photoelectron spectroscopy (XPS), and X-ray diffraction (XRD). Their photocurrent properties of these nanowire electrodes in the photoelectrochemical cell were also investigated

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장소: 제주ICC

발표코드: I-PHYS.P-19

발표분야: 물리화학

발표종류: 포스터, 발표일시: 목 10:30~12:30

## CdS, CdSe Nanocrystals on Nanodiamond as Efficient Photocatalysts

장동명, \*송윤미, 조용재, 김한성, \*\*이치우, 박정희, \*\*\*지아영, \*\*\*이민영

고려대 소재화학과 \*고려대 소재화학과 태양에너지소재 \*\*고려대 신소재화학과 \*\*\*이화여대  
화학나노과학부

Cadmium sulfide (CdS), Cadmium selenide (CdSe) nanocrystals were grown in situ on acid-purified detonation nanodiamonds by a solvothermal method. These various nanocrystal-nanodiamond hybrid nanostructures exhibited excellent photocatalytic activity toward the degradation of methylene blue under visible and UV-visible light irradiation, comparable with corresponding TiO<sub>2</sub> hybrid ones. The great support effect of nanodiamond on photocatalytic activity suggests that the large surface-area of the nanodiamond stabilizes the highly dispersed nanocrystals, and the strong binding interaction between the surface carbon of nanodiamond and the nanocrystals induces efficient interfacial charge transfer to retard electron-hole recombination

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장소: 제주ICC

발표코드: I -PHYS.P-20

발표분야: 물리화학

발표종류: 포스터, 발표일시: 목 10:30~12:30

## Synthesis of PbSSe nanowires using vapor transport method and Their Electrical Transport Properties

장소영, 서영석, 박정희

고려대 소재화학과

Ternary alloy PbSSe nanowires were successfully grown through a one-step thermal evaporation route using Au nanoparticles as a catalyst. They consisted of single-crystalline cubic structure nanocrystal (avg. diameter = 200 nm) grown along the [100] direction. The composition was continuously varied from PbS<sub>0.6</sub>Se<sub>0.4</sub>, PbS<sub>0.2</sub>Se<sub>0.8</sub>, PbS<sub>0.25</sub>Se<sub>0.75</sub>, and PbS<sub>0.08</sub>Se<sub>0.92</sub> using the growth condition. The structure and composition were analyzed using X-ray diffraction, high-resolution transmission electron microscopy, electron diffraction, and energy-dispersive X-ray spectroscopy, showing the consistent values of S and Se composition. We fabricated field effect transistors using single PbSSe NWs, which showed intrinsic p-type semiconductor characteristics for all three routes. This finding may be extended for fabricating other composition-tunable 1D ternary alloy nanostructures.



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장소: 제주ICC

발표코드: I-PHYS.P-21

발표분야: 물리화학

발표종류: 포스터, 발표일시: 목 10:30~12:30

## Synthesis and Characterization of GeBiTe and GeSbTe Nanowires.

정찬수, 박정희

고려대 소재화학과

Solid-state structural transformation coupled with an electronic property change is an important mechanism for nonvolatile information storage technologies, such as phase-change memories. Herein we aim to exploit the phase-change materials of germanium bismuth telluride (GeBiTe) and germanium antimony telluride (GeSbTe) nanowire. High-quality GeBiTe and GeSbTe nanowires have been synthesized via thermal evaporation method under vapor-liquid-solid mechanism. The morphology, chemical composition, and crystal structure of the as-synthesized GeTe-based nanowires were investigated by scanning electron microscopy, energy dispersive X-ray spectroscopy, high-resolution transmission electron microscopy (HR-TEM), and X-ray diffraction pattern. Comparing the phase-change behaviour of GeBiTe to that of GeSbTe, we have tried to verify a general relationship between a metastable cubic and a stable rhombohedral structure.

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발표분야: 물리화학

발표종류: 포스터, 발표일시: 목 10:30~12:30

## **Nano-brambly Cu<sub>2</sub>S forest : room-temperature synthesis and a comparison of vertical aligned Cu<sub>2</sub>S nanowires.**

최진웅, 박정희

고려대 소재화학과

Cu<sub>2</sub>S, with an indirect bandgap of approximately 1.2 eV, is an appealing photovoltaic material. The synthesis of vertically aligned Cu<sub>2</sub>S 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, O<sub>2</sub> 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 Scanning electron microscope(SEM), X-ray diffraction(XRD), Transmission electron microscope(TEM), Raman spectrum.

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## **Zn<sub>1-x</sub>Cd<sub>x</sub>Se ternary alloyed layer sensitized ZnO Nanowire array as Efficient Photoelectrode**

**명윤, 김한성, 박정희**

고려대 소재화학과

High-density complete composition-tuned Zn<sub>1-x</sub>Cd<sub>x</sub>Se alloy layers were deposited on pre-grown ZnO nanowires using by the thermal vapor transport method. Their shell alloy composition controlled by growth temperature and reaction time. The structure and composition of nanocables were analyzed using X-ray diffraction, X-ray photoelectron spectroscopy, high-resolution transmission electron microscopy, energy-dispersive X-ray spectroscopy and UV-visible spectroscopy showing the consistent values of Zn and Cd composition. In addition, we were found that the nanowire arrays have good light absorption characteristics and these properties make it suitable for photoelectrochemical cell.

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발표종류: 포스터, 발표일시: 목 10:30~12:30

## **phase change behaviors of GeSbTe nanowire in electrical memory device**

서영석, 김한성, 조용재, 명윤, 박정희

고려대 소재화학과

Phase-change materials, which can be reversibly switched between amorphous and crystalline states, are promising in this respect, but top-down processing of these materials into nanostructures often damages their useful properties. Self-assembled nanowire-based phase-change material memory devices offer an attractive solution owing to their sub-lithographic sizes and unique geometry, coupled with the facile etch-free processes with which they can be fabricated. Here, we explore the effects of nanoscaling on the memory storage capability of self-assembled GeSbTe nanowires, an important phase-change material.

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발표종류: 포스터, 발표일시: 목 10:30~12:30

## Comprehensive Studies on the Free energies of Solvation and Conformers of Glycine: A Theoretical Study

박병호, 김창곤, 이해황, 김찬경

인하대 화학과

In this work, among all the possible structures of glycine, the seven NE conformers and the inter-conversion between the seven NE forms have been examined in aqueous solution as well as in the gas phase. The structures of the seven NE conformers of glycine and transition structures for inter-conversions between the NE conformers in the gas phase were fully optimized without any geometrical constraints at B3LYP level with 6-311+G(d,p) and 6-311+G(3df,2p) basis sets and MP2 and CCSD level with 6-311+G(d,p) basis set. The energetics were then refined at CCSD(T)/6-311+G(d,p) level on geometries at CCSD/6-311+G(d,p) level. For the conformations in aqueous solution, the seven NE conformer and the ZW conformer were firstly optimized at the CPCM-B3LYP/6-311+G(d,p) level adopting the six cavity models, UA0, UAHF, UAKS, UFF, PAULING, and BONDI models in order to choose the most reliable cavity model. In aqueous solution, the intramolecular proton transfer between the NE and ZW forms have been also investigated for three possible paths (i) direct intramolecular proton transfer, (ii) intramolecular proton transfer participating water molecule(s), and (iii) proton exchange process with water molecule via the anionic intermediate (AN) of glycine and hydronium ion. All calculations were performed with the Int(grid=ultrafine) option by using the Gaussian-03 program.

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발표종류: 포스터, 발표일시: 목 10:30~12:30

## Theoretical Studies on the Effects of Alkali Metal Cations for the Reactions of Phenyl Aryl Chlorophosphates with Anilines and Pyridines and $(\text{OCH}_3)_2\text{P}(=\text{O})\text{Cl}$ with Ammonia in the Gas Phase and in Aqueous Solution

한인숙, 김창곤, 김찬경, 이해황

인하대 화학과

Ab initio molecular orbital calculations at the MP2 level were theoretically examined for the Alkali-Metal Cation,  $\text{X}^+$  ( $=\text{Li}^+$ ,  $\text{Na}^+$ ,  $\text{K}^+$ ), for the substitution reactions of phenyl aryl chlorophosphates,  $\text{C}_6\text{H}_5\text{OP}(=\text{O})(\text{Cl})\text{OC}_6\text{H}_5$ , with aniline and pyridines, and  $(\text{OCH}_3)_2\text{P}(=\text{O})\text{Cl}$  with ammonia in the gas phase and in aqueous solution. All the reactions were found to proceed via a concerted mechanism with the nucleophile(aniline, pyridine and ammonia) and leaving group (Cl) occupying apical sites each other at the transition states (TS). Except for the reactions of  $(\text{OCH}_3)_2\text{P}(=\text{O})\text{Cl}$  without  $\text{X}^+$ , the TSs via a concerted process or any stable intermediates could not be located as stationary point species on the reaction coordinates in the gas phase. This indicates that the effects of  $\text{X}^+$  play a considerably important role. All the stationary point species have been fully optimized and characterized by frequency calculations at MP2 level with 6-31+G(d) basis sets.

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발표분야: 물리화학

발표종류: 포스터, 발표일시: 목 10:30~12:30

## Estimation of Heats of Vaporization of organic molecules using QSPR Method

Li Jun, 김찬경, 김창곤, 이해황, \*조수경

인하대 화학과 \*국방과학연구소 4기술-2-1

One of the most vital properties of organic molecules is the heat vaporization, and the determination of this factor helps to choose proper candidates for even deeper research. But unfortunately the estimation of the property is difficult. In this work, about 50 organic molecules are optimized to minima which were verified from the frequency calculations at the B3LYP/6-31G\* theory level. And 50 descriptors ranging from 0D to 3D molecular structures were generated. Then we did multiple regressions after limiting the number of variables to 5, some reasonable QSPR equations are derived. Further study in this filed about high energetic molecules is still being carried on.

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## Mechanistic Insights into Nickel-Catalyzed Hydroheteroarylation of Vinylarenes

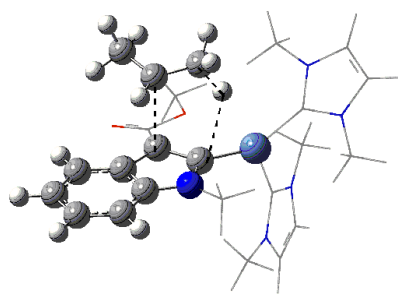
**GAO JIEYING**, su zhishan, \*Ying Xue, \*\*김찬경

인하대 물리화학 \*College of Chemistry, Sichuan University, PR China \*\*인하대 화학과

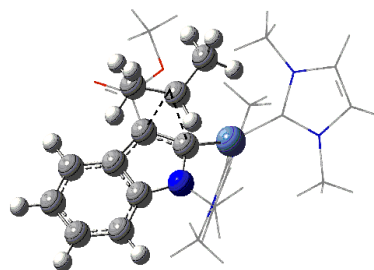
The mechanisms of nickel-catalyzed hydroheteroarylation of vinylarenes were studied by use of computational techniques. Optimized structures for all of the stationary points in the gas phase were investigated using the density functional theory (BP86) method. The SDD pseudopotential, along with its associated basis set, was used to describe the nickel centers, while the 6-31G\* basis set was used for the main group atoms C, O, N, and H. Two distinct possible pathways in the title reaction were evaluated, involving the conventional oxidative addition and the new direct addition, respectively. Furthermore, in each pathway, two types of reaction processes were explored, which leads to 1,1-diarylethane as product and 1,2-diarylethane as product, respectively. Our calculated results indicate that the newly found addition mechanism is more favorable than the conventional oxidative addition due to the strong steric hindrance. The reaction pathway leading to 1,1-diarylethane as product has the higher possibility to occur, with the energy barrier being lower by ca. 9kcal/mol compared with that forming to 1,2-diarylethane as product, which is in good agreement with the experimental observation.



new direct addition



TS1



TS2



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## Kinetics and Mechanism of the Anilinolysis of *p*-*p*-Dicyclohexyl Phosphinic Chloride in Acetonitrile

울혁, \*Adhikary Keshab Kumar, \*\*Hasi Rani, \*김찬경, \*이해황

인하대 물리학과 \*인하대 화학과 \*\*인하대 물리화학과

The reactions of *p*-*p*-dicyclohexyl phosphinic chloride (1) with X-anilines in acetonitrile at 60.0 °C are studied kinetically. The Hammett  $\rho_X$  ( $\rho_{\text{nuc}} = -1.95$ ) and Brönsted  $\beta_X$  ( $\beta_{\text{nuc}} = 0.71$ ) values, and the secondary inverse kinetic isotope effects ( $k_H/k_D = 0.843 < 1$ ) involving deuterated aniline ( $\text{XC}_6\text{H}_4\text{ND}_2$ ) nucleophiles are obtained. The small magnitudes of  $\rho_X$  and  $\beta_X$  values, and secondary inverse DKIEs suggest a concerted  $\text{S}_{\text{N}}2$  mechanism with early transition state (TS) involving predominantly backside nucleophilic attack. Relatively much smaller rates of 1, compared to other chlorophosphinates is rationalized by the steric effects of the cyclohexyl ligands.

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## Kinetics and Mechanism of The Benzylaminolysis of O,O-Dimethyl S-Aryl Phosphorothioate in Dimethyl Sulfoxide

Adhikary Keshab Kumar, \*Hasi Rani, \*\*울혁, 김찬경, 이해황

인하대 화학과 \*인하대 물리화학과 \*\*인하대 물리학과

The interpretation of mechanism with the experimental database of physical behavior of bioactive organo-phosphorus compounds are interesting and important in the field of physical organic chemistry. In the incessant of the progress of experimental physical chemistry the kinetics and its mechanism are usually concern to the physical factors of the relevant compound in the nature. Recently we are studying the mechanistic criteria of benzylaminolysis of O,O-Dimethyl S-Aryl Phosphorothioate in Dimethyl Sulfoxide at 85.0 °C . Usually a biphasic Hammett plot indicates the mechanistic alteration during the change in X or Z-substituents variation of nucleophiles or substrate while acting in the reaction stream or linear correlation for straight forward  $S_N1$  or  $S_N2$  type of mechanistic interpretation. The deuterium kinetic isotope effect is the strong tool for mechanistic interpretation, although respective activation parameters and obtained cross-interaction constants are the main basic information for interpreting mechanism of the system. Where, we are especially endeavored to introduce the frontal and backward attack of nucleophiles through the usual  $S_N1$  or  $S_N2$  nucleophilic substitution reaction. In the present work, It was intended to speculate and provoke the mechanistic criteria and change with the sharp deviation into break of the Hammett and Brönsted linear correlations in the course of reactions mentioned above.

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발표종류: 포스터, 발표일시: 목 10:30~12:30

## Kinetics and Mechanism of The Pyridinolysis of O,O-Dimethyl S-Aryl Phosphorothioate in Dimethyl Sulfoxide

Hasi Rani, \*Adhikary Keshab Kumar, \*\*울혁, \*김찬경, \*이해황

인하대 물리화학과 \*인하대 화학과 \*\*인하대 물리학과

The mechanistic interpretation with its statistical database of physical behavior of organo-phosphorus compounds are appearing as an interesting materials for bioactive and biosensing materials recently in physical organic chemistry. Usually the Hammett and Brönsted plots are indicated the mechanistic criteria during the change in X or Z-substituents variation of nucleophiles or substrate respectively. The nonlinear Hammett and Brönsted plots are the indication of mechanistic change during the course of reactions. The Deuterium Kinetic Isotope Effect (DKIE) is the strong tool for mechanistic interpretation and interpreted primary deuterium kinetic Isotope Effect confers the H-bond effect at the TS. The respective activation parameters and obtained cross-interaction constants ( $\rho_{XZ} = -0.15$  and  $-0.35$ ) with large positive  $\rho_X$  (For 4-NH<sub>2</sub> – H, 1.51 – 1.73 and For H – 4Ac, 0.959 – 1.10),  $\rho_Z$  (For 4-MeO – 4-Cl, 1.05 – 1.35) and  $\beta_X$  (For 4-NH<sub>2</sub> – H, 0.250 – 0.288 and For H – 4Ac, 0.190 – 0.219) are the main basic information for interpreting mechanism. Where, we are especially endeavored to introduce the frontal and backward attack of nucleophiles through the usual S<sub>N</sub>1 or S<sub>N</sub>2 processes. In the present work, we intended to speculate and provoke the concerted S<sub>N</sub>2 mechanism with the early TS from the Cross Interaction Constants, Hammett and Brönsted correlations in the course of reactions mentioned above.

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발표종류: 포스터, 발표일시: 목 10:30~12:30

## Theoretical Investigation on the Mechanism of Michael Addition of Malononitrile to $\alpha,\beta$ -unsaturated ketones Catalyzed by quinidine

su zhishan, \*이해황, \*김찬경

인하대 물리화학 \*인하대 화학과

The mechanism of Michael addition of malononitrile to  $\alpha,\beta$ -unsaturated ketones catalyzed by primary amines derived from quinidine was investigated by DFT method with 6-31+G\* basis set. The computational results indicate that ketone substrates could be activated by generating reactive iminium ion intermediates through primary amine group of quinidine. The tertiary amine in quinidine could work as Lewis base to promote the activation of malononitrile and deprotonation. Two continued stages are involved in the overall reaction; (i) the formation of iminium ion intermediates; (ii) the addition reaction between iminium ion and Malononitrile. The step corresponding to the transfer of H atom from quinoline unite to C atom of ketone was predicted to be the rate-determining step.

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## Ground-State Triple Proton Transfer of 1:2 7-Hydroxyquinoline/Alcohol Complexes: Reaction Dynamics Governed by Configurational Optimization

박선영, 장두전

서울대 화학부

The ground-state proton transfer (GSPT) of 7-hydroxyquinoline along a hydrogen-bonded alcohol chain has been investigated in *n*-alkanes using time-resolved transient-absorption spectroscopy with variation of alcohols, media, isotopes, and temperatures. As a 7-hydroxyquinoline molecule associates with two alcohol molecules via hydrogen bonding to form a cyclic complex in a nonpolar aprotic medium, the intrinsic GSPT dynamics of the cyclic complex in *n*-alkanes has been observed directly without being interfered with by solvent association to form the cyclic complex. The GSPT of the cyclic complex occurs concertedly without accumulating any reaction intermediate and yet asymmetrically with a rate-determining tunneling process. Both the rate constant and the kinetic isotope effect of GSPT increase rapidly with the proton-donating ability of the alcohol but decrease gradually with the molecular size of the alcohol. The hydrogen-bond bridge reorganization of the cyclic complex to form an optimal precursor configuration for efficient proton tunneling takes place prior to intrinsic GSPT, and configurational optimization becomes more important as the molecular size of the alcohol increases. Consequently, the larger contribution of configurational optimization to GSPT leads to the weaker asymmetric character of GSPT.

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발표종류: 포스터, 발표일시: 목 10:30~12:30

## Laser-Induced Synthesis of Au@CdS Core-Shell Nanowires

김종엽, 장두전

서울대 화학부

Au@CdS core-shell nanowires have been fabricated readily by exciting the surface-plasmon resonances of gold nanospheres, which were priorly connected to each other by 1,5-pentanedithiol (PDT) and coated with CdS, using picosecond laser pulses at room temperature. Gold nanospheres were cross-linked by PDT molecules to form gold nanostrands, which were then fixated and protected by CdS shells to yield Au@CdS core-shell nanocomposites. The irradiation of the nanocomposites loaded on a grid of transmission electron microscopy with 532 nm pulses of 30 ps has produced Au@CdS core-shell nanowires. The thermalized photon energy of surface-plasmon excitation has induced gold nanospheres to fuse together within CdS shells.

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발표종류: 포스터, 발표일시: 목 10:30~12:30

## Synthesis and Characterization of Highly Luminescent CdSe@ZnS Core-Shell Nanorods

김형배, 김종엽, 장두전

서울대 화학부

Semiconductor nanocrystals have received much attention for both fundamental research and technical application, due to their strong size dependent properties and excellent chemical processibility. Highly luminescent CdSe@ZnS core-shell nanorods stabilized by mercaptopropionic acid in water were synthesized wet-chemically and characterized by measuring photoluminescence spectra and absorption spectra, diffraction patterns and electron microscope images. By changing the reaction conditions, we have controlled the morphology of CdSe@ZnS core-shell nanoparticles. Photoluminescence from CdSe nanorods shifts to the blue and increases several times with the increase of the ZnS shell thickness. Their strongly enhanced and near-IR fluorescence from CdSe@ZnS core-shell nanorods is attractive for the use of biological applications in cellular labelling, deep-tissue imaging, and biosensing.



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발표종류: 포스터, 발표일시: 목 10:30~12:30

## Facile Hydrothermal Growth Control of Highly Luminescent ZnS Nanobelts

김연호, 김종엽, 장두전

서울대 화학부

Semiconductor nanocrystals with defined size and shape have drawn much attention because of their great potential for fundamental research on the effect of dimensionality for electronic and optoelectronic nanodevice applications. One-dimensional nanocrystals of ZnS such as nanowires, nanorods, nanosheets, and nanobelts have been synthesized with high crystalline quality, showing unique electronic and optical properties because of its wide direct band gap (3.77 eV for the hexagonal wurtzite phase and 3.72 eV for the cubic phase at room temperature). The belt-like nanostructures offer exciting opportunities for both fundamental research and technological applications. By changing the reaction conditions, we have controlled the morphology of ZnS nanocrystals. We will introduce a convenient hydrothermal method to synthesize uniform ZnS nanobelts and optical properties with variation of temperature, reaction time, concentration and characterized by using EDX, FE-SEM, HR-TEM, IR, XRD, and optical spectroscopic methods.

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## **Water-Assisted Highly Efficient Synthesis of Multi- Walled Carbon Nanotubes by Microwave Plasma Enhanced Chemical Vapor Deposition(MPECVD)**

허창순, 이상국

부산대 화학과

We have demonstrated the efficient microwave plasma enhanced chemical vapor deposition(MPECVD) synthesis of multi-walled carbon nanotubes where the activity and lifetime of the catalysts are enhanced by water vapor. Water-stimulated enhanced catalytic activity results in massive growth of superdense and vertically aligned nanotube forests with heights up to 50 micrometers in a 30-min growth time that can be easily separated from the catalysts. Moreover, highly organized intrinsic nanotube structures were successfully fabricated. Although water-assisted synthesis method addresses many critical problems that currently plague carbon nanotube synthesis, we have found that H<sub>2</sub> plasma plays an important role in promoting and preserving catalytic activity. Water assisted growth was successfully carried out on catalysts that generate MWNTs, including Ni nanoparticles from sputtered metal thin films (TiN) on Si wafers, which demonstrates the generality of our approach.

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발표종류: 포스터, 발표일시: 목 10:30~12:30

## Formation of Zn microspheres by a simple way of chemical vapor deposition(CVD)

정승환, 이상국

부산대 화학과

Zn microspheres have been prepared by heating a mixture of ZnO/graphite powders using the chemical vapor deposition(CVD) and vapor transport on Si(1 0 0) substrates without any catalyst. The crystal structure morphologies, transformation, and photoluminescence evolution of the Zn microspheres were studied and investigated with X-ray diffraction (XRD), scanning electron microscopy (SEM), Energy dispersive spectroscopy(EDS), X-ray diffraction (XRD), and photoluminescence (PL) spectra. The room-temperature photoluminescence spectrum (PL) of the as-synthesized Zn microspheres exhibits a weak ultraviolet (UV) emission band centered at 394nm and a strong green emission band centered at 518nm which are assigned to the near band-edge emission and the deep-level emission, respectively. The specific structure of the highly oriented two-dimensional microspheres may find applications in nanoelectronics, nanophotonics and nanomedicine.

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발표종류: 포스터, 발표일시: 목 10:30~12:30

## Vibronic Spectroscopy of p-xylyl radical in the Corona Excited Supersonic Expansion

윤영욱, 이상국

부산대 화학과

The p-xylyl radical was produced in a jet from p-xylene and vibronically excited with a carrier gas(He) in a corona excited supersonic expansion using a pinhole-type glass nozzle. The vibronically resolved emission spectrum of the jet-cooled p-xylyl radical in the D1→D0 transition has been recorded with a long-path monochromator in the visible region. The spectrum was analyzed to obtain accurate electronic transition and vibrational mode frequencies in the ground electronic state by comparing with those from the ab initio calculation as well as those of p-xylene.

일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: I -PHYS.P-40

발표분야: 물리화학

발표종류: 포스터, 발표일시: 목 10:30~12:30

## **DFT study of close-ended tubular boron clusters and their metal complexes I**

장효원

순천대 화학과

Based on the DFT calculations of stable thinnest boron nanotubes reported previously by others, we calculated related stable clusters in which those tubes form loop structures. They are formed by joining building blocks side by side. The circular shaped hexamer is found to be more stable than the pentamer or the heptamer, apparently because of the strains developed when forming rings with given number of building blocks. These loops are slightly more stable than the linear tubes near the hexamer region. We also examined their binding properties with several metal atoms including Be.

일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: I-PHYS.P-41

발표분야: 물리화학

발표종류: 포스터, 발표일시: 목 10:30~12:30

## Observation of Phosphorescent Ir(III) Complexes Inter-ligand Energy Transfer

유효선, 이길용, 안태규, \*박수영

성균관대 에너지과학과 \*서울대 재료공학부

Transition metal complexes are promising material as they offer highly efficient room-temperature phosphorescence. One of the important metal complexes is Ir(III) complexes for electrophosphorescence including light-emitting electrochemical cells (LECs) and organic light-emitting devices (OLEDs). Exothermic interligand energy transfer (ILET) from the cyclometalating ligand to the emitting ancillary ligand by time-resolved spectroscopy, which afforded a novel strategy of emission color tuning. Youngmin You et al., insists the time scale of ILET is 6~7 ns. It was first paper observation of Exothermic interligand energy transfer (ILET). But Taiwan group case, Ir(III) complexes response limited rise (

일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: I-PHYS.P-42

발표분야: 물리화학

발표종류: 포스터, 발표일시: 목 10:30~12:30

## **Photo-induced thermo-acoustic spectrum : Image Reconstruction by different depth**

### 서갑석

성균관대 에너지과학과

Title : Photo-induced thermo-acoustic spectrum : Image Reconstruction by different depth. Photo-induced thermo-acoustic image is emerging as a non-ionizing imaging modality. When electromagnetic radiation is irradiated upon different depth sample, the resulting heat-related expansion of the material produces acoustic waves. From the acoustic signals, we can reconstruct the distribution of electromagnetic absorption in sample. The large differences in electromagnetic absorption in various condition, which are associated with their physiological and pathological status, provide significant contrasts in imaging. So we develop the thermo-acoustic signal from different depth material. 1) 1mm depth iron 2) 0.5mm plastic 3) 0.6mm wood sticFinally. Our different condition and depth sample Easily can make very different vibration. Using that point. Make sure this depth and make reconstruct image.

일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: I-PHYS.P-43

발표분야: 물리화학

발표종류: 포스터, 발표일시: 목 10:30~12:30

## Origins for Selective Reactivity of Tridentate Macrocycles in Square Planar Pd([9]aneA<sub>2</sub>B)Z<sub>2</sub> Complexes

최호준, \*구인선, \*박종근

경상대 화학과 \*경상대 화학교육과

The relative stability for the coordination bond of tridentate nine-membered macrocycles {[9]aneA<sub>2</sub>B), ([9]aneABA)} to PdZ<sub>2</sub> and the fluxional variation of the geometric configuration for distorted Pd complexes were investigated using DFT methods. To get the more preferential interaction among the soft A (or hard B) atom, the selective coordination reaction between the d<sub>x<sup>2</sup>-y<sup>2</sup></sub>-orbital and the lone pair electron of A (or B) have been investigated along the lower transition coordinate. To investigate the fluxional variation of the square-planar geometry, the stable isomers were optimized. Because of the vacant space on the Z-axis, the geometric configuration were easily changed from the apical (B...Pd) interaction to the basal direction. Along the atomic configuration coordinate, the order and energy gap of molecular orbital in each step were not deformed by the orbital interaction and geometric change.



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장소: 제주ICC

발표코드: I-PHYS.P-44

발표분야: 물리화학

발표종류: 포스터, 발표일시: 목 10:30~12:30

## Analysis of Raman spectra for an organic/inorganic hybrid gel

이호익, 이성영, 손대원

한양대 화학과

A hydrogel is a material that has a 3D network structure which could be obtained using radiation, ion beam, chemical crosslinker, or physical interactions. We synthesized the hydrogel and investigated Raman activity of Imogolite hybrid hydrogel. Imogolite is a natural, hydrated aluminium silicate with a hollow tube structure. We find characteristic peaks of pAA, C-H and C=O stretching around 1400  $\text{cm}^{-1}$  and 1700  $\text{cm}^{-1}$  in hybrid Imogolite hydrogel. Imogolite nanotubes mainly contribute to the range of under 1200  $\text{cm}^{-1}$  in Raman spectra. This result is similar with simulated Raman spectra. We are using the model of pure and hybrid imogolite cluster with small and large imogolite. In addition, we have investigated Raman spectra with respect to the length of pAA chain. In result, we figure out the peak around 850  $\text{cm}^{-1}$  originated from the bond between pAA and Imogolite nanotubes. And the intensity around 1400  $\text{cm}^{-1}$  is enhanced for the long chain of pAA. Therefore, we can successfully explain the characteristic peaks of experimental Raman spectra.

일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: I -PHYS.P-45

발표분야: 물리화학

발표종류: 포스터, 발표일시: 목 10:30~12:30

## **Influence of Nonlinear Configuration in Charge Transfer Processes**

최완, 심은지

연세대 화학과

We investigate configuration dependent charge transport processes of nonlinear donor-bridge-acceptor system using the on-the-fly filtered propagator functional path integral(OFPF-PI) approach. The OFPF-PI method dramatically reduces the forward-backward pair trajectory space to be integrated without losing numerical accuracy by filtering negligible propagator elements at each propagation step. In order to employ nonlinear configuration of the model system, we reformulate the OFPF-PI method. Extension of the reaction coordinate to multi-dimensional degrees of freedom allows to accounting for various configurations of the system as well as the complex characteristics of the electronic interaction. We discuss influence of the configuration on the dynamics of quantum transfer processes.

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장소: 제주ICC

발표코드: I-PHYS.P-46

발표분야: 물리화학

발표종류: 포스터, 발표일시: 목 10:30~12:30

## Determination of degree of coherence through effective electronic coupling

이지혜, 김희영, 심은지

연세대 화학과

We investigated relationship between electronic coupling constant and the coherence length for quantum transfer systems. The reduced density matrix of the transfer processes is evaluated by means of a reduced trajectory space analysis combined with the on-the-fly filtered propagator functional path integral formalism. Quantitative estimation of the coherence length is important due to its close relationship to charge transfer mechanism and, thus, can give crucial information on designing molecular electronic devices. It was found that coherence length depends on the number of indiscrete strong electronic couplings in long-range quantum transfer. By employing a simple three-state donor-bridge-acceptor model, we found that the effective coupling formula which can be used to estimate the degree of coherence of the charge transfer dynamics. In this presentation, the effective coupling formula and the criterion the degree of coherence are discussed.

일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: I-PHYS.P-47

발표분야: 물리화학

발표종류: 포스터, 발표일시: 목 10:30~12:30

## **pH-sensitive Structure Change of Self-assembled AB<sub>2</sub> Miktoarm Star Copolymers**

홍민형, 심은지

연세대 화학과

Dissipative particle dynamics simulations were performed to study pH-sensitivity of onion-like multi-layered structure formed from self-assembly of AB<sub>2</sub> miktoarm star copolymers. AB<sub>2</sub> miktoarm star copolymer is modeled with a flexible bead-spring coarse-grained molecule which consists of a hydrophilic A segment and two hydrophobic B segments. Balanced repulsion between the head group and solvents provides an effective confined environment and gives rise to multi-layered micelle secondary structure. We discuss structural change of the multi-layered micelle due to solvent pH change. In the view of drug vehicles, onion-like multi-layered structure maybe useful, particularly for extended drug release, hydrophobic drug molecules can be efficiently encapsulated by the hydrophobic domain. Efficacy of the multi-layered structure is also discussed in comparison to that of similar size vesicles or spherical micelles.

일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: I-PHYS.P-48

발표분야: 물리화학

발표종류: 포스터, 발표일시: 목 10:30~12:30

## Diffusion of Iodine in Ionic Liquid-based Electrolyte for DSSC systems: Role of Water Contents

전지원, \*김형준, \*\*이가인, \*\*\*William A.Goddard III

KAIST EEWS \*KAIST EEWS 대학원 \*\*KAIST 신소재 \*\*\*California Institute of Technology

A dye-sensitized solar cell (DSSC) is an attractive device because of its relatively low-cost solar energy conversion. One key mechanism of the DSSC operation is the oxidation/reduction reactions of I-/I<sub>3</sub><sup>-</sup> ions in the electrolyte, and their faster diffusion is important to achieve a better efficiency. On the other hand, device stability under electrochemical cycles and temperature variations is a critical issue for the actual application of DSSC. Imidazolium based ionic liquid has been regarded as a better electrolyte than the acetonitrile based one in terms of device stability, but the efficiency is ~5% which is lower than the world record of ~11% measured in acetonitrile based electrolyte. Here, we investigate the role of water molecules in the ionic liquid, which has been thought as negative because it can degrade dyes from TiO<sub>2</sub> surface. First principle based force-field parameters are prepared using quantum mechanical (QM) simulations, then molecular dynamics (MD) simulations are performed to understand the kinetics of electrolytes. We find that small amount of water molecules can efficiently screen the coulomb interactions of I<sup>-</sup> ions, making them more mobile in the solution. We further discuss the optimal amount of water to maximize the transport of I<sup>-</sup> with minimizing the device degradation.

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장소: 제주ICC

발표코드: I-PHYS.P-49

발표분야: 물리화학

발표종류: 포스터, 발표일시: 목 10:30~12:30

## Self-interaction-free Density Functional Electron Affinities on Molecules: Finding Approximate functionals on Hartree-Fock Density.

김민철, 심은지, \*Kieron Burke

연세대 화학과 \*University of California, Irvine

Electron affinity (EA) calculations with traditional density functional theory (DFT) suffers from self-interaction error, which results in positive HOMO energy levels, and therefore cannot bind electrons in large basis set limits. We prevent this problem using a recently proposed scheme assessing DFT energy on Hartree-Fock (HF) densities[1]. In this talk, we show adiabatic EAs of molecules evaluated from DFT upon traditional Kohn-Sham densities and HF densities. Structure and energy of neutral and anionic species in the G2-1 set[2] are calculated with the PBE, PBE0, and B3LYP functionals. For each approximate functional, self-interaction-free DFT energies are estimated upon HF densities. Comparing the mean absolute error between calculated EA and experimental EA, EA from HF density derived DFT (HF-DFT) gives better results than the traditional DFT. Furthermore, HF-DFT gave negative HOMOs indicating converged results. For molecules like CN, however, HF-DFT fails to give accurate EA due to the poor description of HF density. All calculations were performed with the Turbomole 6.2 program package. [1]D. Lee, F. Furche, K. Burke, J. Phys. Chem. Lett. 2010, 1, 2124-2129.[2]L. A. Curtiss, K. Raghavachari, G. W. Trucks, J. A. Pople, J. Chem. Phys. 1991, 94, 7221-7230.

일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: I-PHYS.P-50

발표분야: 물리화학

발표종류: 포스터, 발표일시: 목 10:30~12:30

## Phase Diagram of Surface Tethered Polymer Sheet in a Dilute Solution

한민우, 심은지

연세대 화학과

A phase diagram of surface tethered polymer sheet in a dilute solution is investigated by using dissipative particle dynamics (DPD) method. To construct a tethered surface, flexible linear coils are attached on the surface of the sheet by harmonic springs. Also, the sheet stiffness is applied by using additional angle potentials. Changing the coil-solvent interaction and sheet stiffness induces various morphologies including hollow and scrolled tubular structures. Theoretically, tubular structures have been predicted with two-dimensional anisotropic sheets with long-range orientational order. By introducing surface tethered model, however, we could obtain two different phases of tubular structures. The governing factor is the sheet curvature which is caused from coil-solvent interaction asymmetry between upper and lower side of the sheet and the sheet stiffness. The curvature becomes larger when higher asymmetry applied so that scrolled tubular structures are observed. While, the hollow tubular structures appear from the sheet with smaller curvature when higher sheet stiffness applied. We found that the surface tethers play a significant role to determine the sheet morphologies and previous experimental results shows same reasonable agreement.

일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: I-PHYS.P-51

발표분야: 물리화학

발표종류: 포스터, 발표일시: 목 10:30~12:30

## **Infrared predissociation spectroscopy of aniline-water-pyrrole cluster cation : The evidence of mode selectivity**

**MD.ALAUDDIN, 송재규, 박승민**

경희대 화학과

The vibrational gas phase spectrum of aniline-water-pyrrole cluster cation (AWP+) has been measured by using infrared predissociation spectroscopy (IR/R2PI). To understand the factors such as intermolecular hydrogen bonding, Van der Waals bonding, energetic effect, size effect and kinematic effect which play key roles in determining the branching ratio of concurrent predissociation reaction. The major photofragment in the IR predissociation of AWP+ was AP+ which led us to conclude that not only energetic but also size and kinematic effects play a important role in determining the liberation of solvent molecule. The branching ratio was slightly dependent on the specific excited mode and the most effective mode to liberate water was free NH vibration of aniline.



일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: I -PHYS.P-52

발표분야: 물리화학

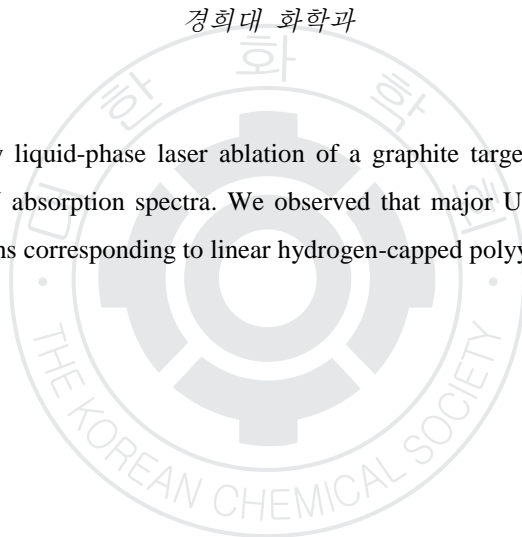
발표종류: 포스터, 발표일시: 목 10:30~12:30

## **Preparation of polyynes by liquid laser ablation of graphite target at various solvents and wavelength**

박영은, 신승근, 송재규, 박승민

경희대 화학과

Polyynes were prepared by liquid-phase laser ablation of a graphite target at various wavelength and identified by analyzing UV absorption spectra. We observed that major UV absorption peaks coincide with the electronic transitions corresponding to linear hydrogen-capped polyynes ( $C_nH_2$ :  $n = 8, 10$ ).



일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: I-PHYS.P-53

발표분야: 물리화학

발표종류: 포스터, 발표일시: 목 10:30~12:30

## **Preparation of TiN films by Laser Ablation of Ti Target in N<sub>2</sub> atmosphere**

정다운, 신승근, 송재규, 박승민

경희대 화학과

The chemiluminescent reaction between Ti atoms produced by pulsed laser ablation (PLD) in nitrogen atmosphere. The TiN plasma plume is produced by using a Nd:YAG laser (266nm) and deposited on the silicon wafer substrate in presence of magnetic field. We have studied this deposited films by using Raman spectroscopy. The optical properties of the deposited TiN films were measured by using photoluminescence (PL) spectroscopy at room temperature.

일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: I-PHYS.P-54

발표분야: 물리화학

발표종류: 포스터, 발표일시: 목 10:30~12:30

## Investigation of magnetic properties of $[\text{Cu}_2(\text{MoO}_4)_2(3,4'\text{-dpk})(\text{H}_2\text{O})]$ on the basis of spin dimer analysis

강은비, 구현주

경희대 화학과

The spin exchange interactions of  $[\text{Cu}_2(\text{MoO}_4)_2(3,4'\text{-dpk})(\text{H}_2\text{O})]$  (dpk:dipyridylketone) were examined by using spin dimer analysis on the basis of Extend Hückel Tight Binding (EHTB) method. The crystal structure of  $[\text{Cu}_2(\text{MoO}_4)_2(3,4'\text{-dpk})(\text{H}_2\text{O})]$  is refined in the monoclinic space group  $P2_1/c$  with lattice parameters  $a=10.3911 \text{ \AA}$ ,  $b=6.9502 \text{ \AA}$ ,  $c=22.958 \text{ \AA}$ , and  $\beta=100.658^\circ$ . Our analysis for  $[\text{Cu}_2(\text{MoO}_4)_2(3,4'\text{-dpk})(\text{H}_2\text{O})]$  shows that there are two strongly interacting spin exchange paths  $J_2$  and  $J_4$ . The spin exchange path  $J_2$  consists of two Cu(2) ions in the structural tetramer unit, while the path  $J_4$  is made up of Cu(1) and Cu(2) ions provided from two different structural tetramer units. These two strongly interacting spin units  $J_2$  and  $J_4$  form an isolated  $J_2\text{-}J_4\text{-}J_2$  tetramer chain unit which is not consistent with the structural Cu(1)-Cu(2)-Cu(2)-Cu(1) tetramer unit.

일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: I -PHYS.P-55

발표분야: 물리화학

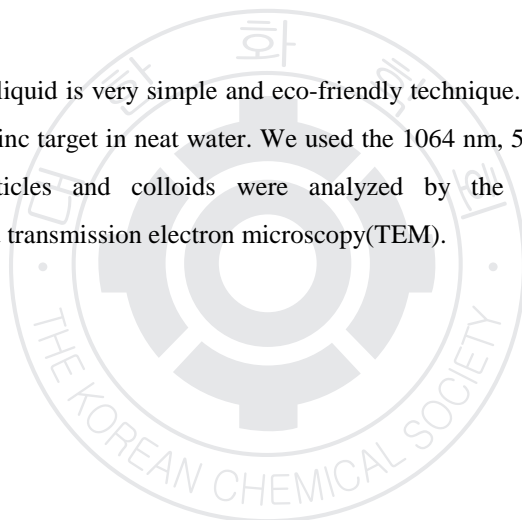
발표종류: 포스터, 발표일시: 목 10:30~12:30

## Wavelength effects on laser ablation of Zn target in neat water

김국기, 신승근, 송재규, 박승민

경희대 화학과

Laser ablation synthesis in liquid is very simple and eco-friendly technique. ZnO nanoparticles produced by pulse laser ablation of Zinc target in neat water. We used the 1064 nm, 532 nm and 355 nm Nd:YAG laser. The ZnO nanoparticles and colloids were analyzed by the UV-Vis spectrophotometer, photoluminescence(PL) and transmission electron microscopy(TEM).



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장소: 제주ICC

발표코드: I-PHYS.P-56

발표분야: 물리화학

발표종류: 포스터, 발표일시: 목 10:30~12:30

## **Influence of interpolymer complexation and matrix rigidity on the excited state dynamics of 9-dicyanovinyljulolidine**

지아영, \*이혜민, 이민영

이화여대 화학나노과학부 \*이화여대 화학나노학과

The fluorescence quantum yield of 9-dicyanovinyljulolidine (DCVJ) is very low in fluid solution, but increases markedly in polymer because medium rigidity slows down the internal motion. In this work, we investigated the molecular rotor dynamics of DCVJ in the polymer blends of poly(ethylene oxide) (PEO) and poly(acrylic acid) (PAA). PEO and PAA form a favorable interpolymer complex through hydrogen bonding. We observed that the fluorescence decay times of DCVJ were strongly affected by the molar ratios of the blends and molecular weights of polymers. Based on the observed fluorescence lifetimes, we attempted to delineate the twisting rate process of DCVJ in terms of polymer rigidity. Conclusively, our results show that the elastic modulus governs photoisomerization dynamics in rigid media.

일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: I-PHYS.P-57

발표분야: 물리화학

발표종류: 포스터, 발표일시: 목 10:30~12:30

## Photoisomerization dynamics of 3,3'-diethyloxacarbocyanine in oligo(ethylene glycol)

이혜민, \*이민영

이화여대 화학나노학과 \*이화여대 화학나노과학부

Solvent influence on photoisomerization dynamics has been investigated for several decades. Surprisingly, the use of a homologous series of oligo(ethylene glycol) has never been acknowledged for this purpose. In this work, we have investigated the excited-state dynamics of 3,3'-diethyloxacarbocyanine iodide (DOCI) in oligo(ethylene glycol)s, structured as  $\text{H}[\text{O}-\text{CH}_2-\text{CH}_2]_n\text{-OH}$  ( $n = 2, 3, 4, 5, 6, 7, 8, 10, \text{ and } 12$ ) and their water mixtures. An interesting feature of DOCI and oligo(ethylene glycol)s is that their molecular sizes are comparable, thus the validity of the Kramers-Hubbard relation can be unambiguously tested. In addition, the photoisomerization dynamics of DOCI in newly explored solvent systems are elucidated considering specific solute-solvent interaction, polarity effect, mechanical and dielectric friction.

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발표코드: I-PHYS.P-58

발표분야: 물리화학

발표종류: 포스터, 발표일시: 목 10:30~12:30

## Universal Correction of Dispersive Interactions in Density Functional Theory: New DFT-lg Model

최정모, \*김형준, \*\*William A. Goddard III

KAIST 화학과 \*KAIST EEWs 대학원 \*\*California Institute of Technology

In many biological and energetic materials, van der Waals (vdW) interactions play an essential role. However, density functional theory (DFT) usually fails to predict physical and chemical properties of materials whose interactions are dominated by long-range vdW attractions, because of dynamical corrections between fluctuating charge distributions. To compensate this critical error (with little additional expenses), people have been developed simple correction methods by adding a pairwise dispersion potential to the conventional Kohn-Sham DFT energy (referred as a DFT-D approach). Recently, Liu et al. [J. Phys. Chem. Lett. 1, 2550 (2010)] suggested a DFT-low-gradient (DFT-lg) model with a proper long-range  $1/R^6$  London dispersion interaction at long distances while delivering low gradients at normal valence distances. However, the model has been restricted only for hydrocarbon materials since there has been no systematic way to generalize pairwise interactions of all atom pairs. Here, we suggest a new DFT-lg model having only a single universal scaling parameter (regardless of atoms), so that we can easily extend the application range of the model to cover the whole periodic table. We show that our method whose universal scaling parameter is optimized only for benzene dimers can predict the binding energies of other weakly bound molecular crystals within a chemical accuracy, confirming the universality of our method. Furthermore we investigate the crystal binding energy of actinide fluorides, which has been unattainable from any other methods.

일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: I-PHYS.P-59

발표분야: 물리화학

발표종류: 포스터, 발표일시: 목 10:30~12:30

## **Analysis of Photosynthesis Energy Transfer Process in Core complex Using Complex Network Theory**

이은, \*안태규

성균관대 에너지과학 \*성균관대 에너지과학과

The photosynthetic apparatus in higher plants is designed to perform efficient harvest sunlight and transfer excitation energy to the reaction center (RC). It can be a good model for solar energy conversion technology. If we are able to know about the principle of excitation energy transfer process more specifically in photosynthesis, we will get a insight for total system of photosynthesis. For these reasons, there have been many tries to solve the mysteries in process of excitation energy transfer in photosystems especially in core complex of photosystem II which has the center place gaining the electron by water splitting. But until now there is no conclusion about the excitation energy transfer process in core complex. Since it has the limits in experimental facilities and heavy calculations. So in this research we tried to make an alternative approach to solve the principle of efficient energy transfer process. First of all, we assume the chlorophyll pigments to be point dipoles in core complexes containing reaction centers and establish the theoretical models based on Förster Energy Transfer Equation and Excitation coupling relations. Secondly, by using the 'Complex Network Theory' we have constructed the model of chlorophyll energy transfer and chlorophyll's energy transfer relation network and we have analyzed the network structure. We have calculated centrality, robustness, betweenness and clustering etc. It will allow us to understand about the characteristics of structure of core complex structure in the view of excitation energy transfer.



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## **Non-Michaelis-Menten single-molecule kinetics and geminate recombination effect**

양성은, 성재영

중앙대 화학과

Experimental evidence of the non-Michaelis-Menten (non-MM) kinetics has been observed in several important catalytic reactions, such as the binding of CO to heme in mutated yeast cytochrome c. The combination times turn out to be nonlinear with respect to the substrate concentration, when the observed rates are converted to Lineweaver-Burk plots. The deviation from MM kinetics is especially manifested at sufficiently low substrate concentration, where the diffusive encounter between enzyme and substrate becomes rate-limiting and the subsequent turnover step is relatively faster. In this regard, the geminate recombination of substrate to enzyme can provide a mechanism to explain the non-MM behavior. Based on the novel chemical kinetics presented in our previous study, we take the geminate effect into account by using a modified reaction time distribution of the enzyme-substrate encounter step. We show that plots of the Michaelis-Menten constant with respect to substrate concentration, calculated by the present theory including the geminate effect, provide a satisfactory fit to the experimental data with just a few adjustable parameters.

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발표종류: 포스터, 발표일시: 목 10:30~12:30

## Synthesis of Metallic RuO<sub>2</sub> Nanowires

이유민, \*김명화

이화여대 화학나노과학과 \*이화여대 화학 나노과학과

We report the synthesis of highly crystalline ruthenium dioxide (RuO<sub>2</sub>) nanowires by an atmospheric pressure chemical vapor deposition. The RuO<sub>2</sub> nanowires were grown on a 200 nm silica covered Si (001) wafer, by atmospheric pressure and vapor transport at 650°C, without the use of catalyst. The structural characterization shows that the nanowires have single crystalline properties without any amorphous layers or defects. The structures and morphologies were examined using scanning electron microscopy (FE-SEM), high resolution electron microscopy (HRTEM), X-ray diffraction (XRD) spectrum and Raman spectroscopy. FE-SEM and HRTEM images of the as-grown RuO<sub>2</sub> nanowires on a Si substrate synthesized by a simple vapor transport of RuO<sub>2</sub> powder indicate a high density of RuO<sub>2</sub> nanowires more than 10 μm long and the diameter of each nanowire is ~100 nm. According to XRD spectrum, HRTEM and Raman spectrum, Growth direction determination of a single RuO<sub>2</sub> nanowire is the [001] crystallographic direction and confirm that the phase of the nanowires are tetragonal structure. The electrical measurements show that the RuO<sub>2</sub> nanowires have extremely low resistivity of  $62.5 \pm 8.8 \mu\Omega\cdot\text{cm}$ , uniform electrical materials characteristics with the size distribution. By passing high current ( $>107\text{A}/\text{cm}^2$ ) through the nanowires, very small nanogaps of less than 5 nm are produced, explained by a heuristic model, in which electromigrative and diffusial effects are included.

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## Study of gas storage capacity with surface modified imogolites

전양준, 이지선, 손대원

한양대 화학과

Imogolite is a single-walled aluminosilicate nanotube which is composed of six membered aluminum hydroxide rings having identical structure with layer of gibbsite. The general formula of imogolite is  $\text{Al}_3\text{O}_3\text{SiO}_2\cdot 2\text{H}_2\text{O}$ . Because of Al-OH group on the surface of imogolite, imogolite has hydrophilic property and hydrogen bonding. In general imogolite exists as a bundle. An amphiphilic molecule, octadecylphosphonic acid (OPA) was used to separate the bundle. The modified imogolite with OPA (OPA-imo) is characterized by IR, XRD and STM. The obtained evidences indicated that the alkyl chains of OPA were successfully absorbed on the surface of IMO. The capacity of gas storage for imogolite and OPA-imo is measured by high-pressure apparatus (HP, Bel Japan, INC.) using  $\text{H}_2$  and  $\text{CO}_2$  gases.

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발표종류: 포스터, 발표일시: 목 10:30~12:30

## Dynamics of the $\text{CH}_3 + \text{OH}$ Reaction

이종백, \*김유항, \*\*H. K. Shin

전남대 화학교육과 \*인하대 물리화학부 \*\*Dept of Chem Univ of Nevada

Dynamics of the  $\text{CH}_3 + \text{OH}$  reaction have been studied over the temperature range of 300 – 2500 K by solving the equations of motion for the potential energy composed of rigorously formulated short-range and long-range interactions. Many trajectories ( $\sim 20\%$ ) undergo collision-induced OH dissociation in a direct-mode mechanism on a subpicosecond time scale ( $\sim 10^{-10} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ ). Less than 10% of  $\text{CH}_3 + \text{OH}$  collisions lead to the formation of excited intermediates  $\text{CH}_3\text{OH}^\dagger$  with excess vibrational energies in CO and OH bonds. A small fraction of  $\text{CH}_3\text{OH}^\dagger$  stabilize to  $\text{CH}_3\text{OH}$  with  $k_{\text{CH}_3\text{OH}} 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ , dissociate back to reactants by collision, or form one of various products after intramolecular energy redistribution, which lead to bond dissociation and formation on the time scale of 50 – 100 fs. The principal product is  $\text{CH}_2$  ( $k_{\text{CH}_2}$  being  $10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ ), whereas  $k$ 's for  $\text{CH}_2\text{O}$  and  $\text{CH}_2\text{OH}$  are  $10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ . The minor products are  $\text{HCOH}$ ,  $\text{CH}_3\text{O}$  and  $\text{CH}_4$ , their  $k$ 's being  $10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ . The total rate constant for  $\text{CH}_3 + \text{OH} \rightarrow \text{CH}_3\text{OH}^\dagger \rightarrow \text{products}$  is  $10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  and is weakly dependent on temperature.

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## Reconstitution of major light harvesting complex into giant unilamellar vesicles studied by time-resolved fluorescence spectroscopy

이길용, \*안초희, \*김성규, 안태규

성균관대 에너지과학과 \*성균관대 화학과

We have built an artificial entity mimicking thylakoid from Giant Unilamellar Vesicles(GUVs) which come close to that of biological thylakoid. The artificial thylakoid is composed of a bilayered phospholipid membrane and a transmembrane protein in a vesicular or a 2-dimensional lamellar structure. The vesicles are made by electroformation methods and the 2-dimensional lamellar membrane is made either by using a Langmuir-Blodgett method or by transforming the vesicles on a mica surface. The protein we have studied most is the light-harvest center II (LHC-II), which collects solar energy in photosynthesis. We compare fluorescence lifetime behaviors of a wild type LHC-II with those of mutant proteins which have different xanthophyll compositions. The investigated results are used to explain the photoprotection mechanism of nonphotochemical quenching process(NPQ) in the photosynthetic process of LHC-II

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## **Spatial investigating chlorophyll fluorescence lifetime of PSI and PSII in individual plant cell using fluorescence lifetime imaging microscopy**

김은철, \*김근돈, \*유상동, 안태규

성균관대 에너지과학과 \*SKKU

Photosynthetic light reactions in plant chloroplasts are suitable for spectroscopic (fluorescence) study because those undergo energy transfers from chlorophyll a to reaction center complexes. The fluorescence measurement using plant leaf organs has been developed and studied more than 30 years(Kitajima and Butler, 1975; Munday and Govindje, 1969). Recent developments of fluorescence life-time imaging microscopy further enable to study time-resolved fluorescence (TRF) at a cellular level(Borst and Visser, 2010). However, it is still not so straight forward to acquire and interpret the data from intact leaf tissues due to the interference in cell walls for fluorescence measurements. Thus, little is known for TRF by chlorophyll a that is the key light energy absorbing pigment in plant chloroplasts. To explore energy transfer scheme during photosynthesis with TRF analysis, we applied the protoplasting technique and isolated leaf mesophyll cells without cell walls(Yoo and Cho et al., 2007) and quantitatively measured chlorophyll fluorescence lifetime(CFL). And we analyzed lifetime components which include information about ratio of pigments, which are mainly PSI and PSII on thylakoid membrane. In this study we spatially revealed CFLs of PSI and PSII and observed state transition of photosynthetic apparatus.

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## Isomerization and dissociation of the acrylonitrile molecular ion : A theoretical study

정선화, 임민경, 최중철

동국대 화학과

We have explored the potential energy surface (PES) for the isomerization and dissociation of acrylonitrile molecular ion by quantum chemical calculations at the HF/6-311G(d,p), B3LYP/6-31G(d), CBS-QB3, and CBS-APNO level. The structures of about 20  $C_3H_3N^{+}$  isomers were optimized and their isomerization pathways were obtained. The dissociation pathways for the loss of  $H\cdot$ ,  $H_2$ , and HCN from the acrylonitrile ion were obtained. Based on the PES obtained, the dissociation kinetics will be discussed.

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## Theoretical studies on the metal ion complexation of pentazole and oxopentazole anion

강인숙, 양기열, \*이해황, \*\*조수경

경상대 화학교육과 \*인하대 화학과 \*\*국방과학연구소 4기술-2-1

Among the many polynitrogen compounds, pentazole anion has received considerable attention as promising high energy density materials (HEDM) because of the large bond energy and the aromaticity of the pentazole anion ( $N_5^-$ ). We have performed the computation on the metal ion complexation of nitrogen clusters such as pentazole and oxopentazole by using ab initio and density functional theory (DFT) calculations in the gas phase and in polar solution. Theoretical complexation energies, enthalpies and free energies are estimated, and the structures corresponding to local and global minimum are also reported. In addition, the transition structures along the decomposition pathway to  $(O)-N_3^- + N_2$  molecules were characterized in order to discuss the kinetic stability of the metal-nitrogen clusters.



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## **The facile method to prepare nanostructured bulk hetero-junction solar cells with AAO template**

박종배, \*김성규, 배태성, \*\*윤형중, \*\*서정혜

한국기초과학지원연구원 전주센터 \*성균관대 화학과 \*\*한국기초과학지원연구원 물성과학연구

부

The regioregularity poly(3-hexylthiophene) (RR-P3HT) and the [6,6]-phenyl-C61-butyric acid methyl ester(PCBM) as an active materials have been widely used for bulk hetero-junction solar cells. Generally, the solar cell performance such like a movement of a charge separation and a charge collection was influenced by a polymer packing order and thickness. Usually, crystal plane of RR-P3HT/PCBM is located perpendicularly to electrodes and thickness of RR-P3HT/PCBM has a limited in bulk hetero-junction solar cells. The closer RR-P3HT/PCBM to the electrodes, the more efficiency of solar cell performance will be expected. To increase solar cell performance, we introduced nanostructure for bulk hetero-junction solar cells. Using nanostructure of RR-P3HT/PCBM or electrodes with an anodic aluminum oxide (AAO) as a template, nanostructured bulk hetero-junction solar cells can be formed. The AAO with a ~50 nm average pore diameter and various lengths was used for metallic nanorods synthesized. We will present a facile method to prepare a nanostructure of RR-P3HT and PCBM with Ag nanorod arrays for bulk hetero-junction solar cells.

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발표종류: 포스터, 발표일시: 목 10:30~12:30

## **Fabrication of silver colloid clusters for Surface-enhanced Raman Scattering by immobilizing colloid particles on poly(4-vinyl pyridine) films**

이수연, 서정쌍

서울대 화학부

We have developed a simple method to fabricate silver colloid clusters for surface-enhanced Raman scattering (SERS) by immobilizing colloid particles on poly(4-vinyl pyridine) (PVP) films. PVP was spin-coated on a microscope cover glass. When the PVP-coated cover glass was put in a Petri dish containing a silver colloid solution, colloid particles were immobilized on the PVP film. The number of the immobilized colloid particles increased with increasing putting time, and most of them were isolated. Further, the formation of silver colloid particle clusters occurred following a three-step process: immobilizing colloid particles on the cover glass coated with PVP, adsorbing molecules on the immobilized particles, and then immobilizing colloid particles again. A good SERS spectrum was observed from the colloid clusters by excitation with a 514.5 nm laser line. The calculated enhancement factor on the colloid clusters optimized in size was approximately  $1 \times 10^6$ , which is about 80 times higher than that measured without doing the second immobilization. Our method is relatively simple and inexpensive with respect to fabricating SERS substrates.

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## NMR and DFT Study on Structure and Electronic Properties of Porphyrin Analogues

이미정, Mannix Balanay, 이상희, 김동희

군산대 화학과

We studied  $\beta$ - and meso-substituted porphyrin dyes for dye-sensitized solar cells having a donor- $\pi$  bridging-acceptor system. The dyes were assessed using 1-D and 2-D NMR spectroscopy and theoretical approach. DFT and TD-DFT were employed to calculate geometrical structures, NMR chemical shifts, and electronic properties. The calculated chemical shifts matched well with the  $^1\text{H}$  and  $^{13}\text{C}$  NMR chemical shifts in DMSO- $d_6$ . The changes in  $^1\text{H}$  and  $^{13}\text{C}$  NMR chemical shifts in line with the  $\beta$ -substituents of the porphyrin analogues could be used to determine the directionality of the system which is an important property in photovoltaic applications. Various range-separated exchange-correlation functionals were used to assess the applicability of the method to calculate excited-state energies of the analogues. Polarizability and hyperpolarizability were also calculated to determine the charge transfer of the analogues in consideration.

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## Identifying the Growth direction of V-shaped Ruthenium dioxide nanowires by polarized Raman scattering spectroscopy

이재연, \*이유민, \*\*김명화

이화여대 화학·나노과학과 \*이화여대 화학·나노과학과 \*\*이화여대 화학·나노과학과

Recently, polarized Raman scattering measurements have been used to determine a single nanowire's growth direction. We present polarized Raman scattering results of ruthenium dioxide (RuO<sub>2</sub>) nanowires, especially, V-shaped ones. RuO<sub>2</sub> nanowires have a great potential as materials for electrodes in electrochemical devices and field-emission displays due to their high electrical conductivity, chemical stability, and characteristics for a good diffusion barrier. RuO<sub>2</sub> nanowires were grown on Si wafer by APCVD at about 750 °C without any catalyst. The structures and morphologies were examined using scanning electron microscopy (FE-SEM) and high resolution electron microscopy (HRTEM). The diameter of each nanowire is ~ 200 nm and the length is ~ 2 μm. In a certain condition, most of nanowires are grown to have a V-shape and an angle between the two branches is approximately 52° which is the same for all V-shaped nanowires. We measured polarized Raman spectra of the V-shaped nanowires. RuO<sub>2</sub> is known to have the tetragonal rutile structure with the space group D<sub>4h</sub> - P4/mmm, and two molecular units per primitive cell. Group theory predicts that its Raman active modes belong to the A<sub>1g</sub>, B<sub>1g</sub>, B<sub>2g</sub> and E<sub>g</sub> representations. We observed A<sub>1g</sub>, B<sub>2g</sub> and E<sub>g</sub> Raman active modes and each branch of a V-shaped RuO<sub>2</sub> nanowire grows into [002] direction, respectively. We confirmed the growth direction of a V-shaped nanowire by using HRTEM. We show that polarized Raman scattering spectroscopy can provide a relatively simple and prompt mean to determine the growth direction of a single nanowire, compared to HRTEM.

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## Measurement of stiffness of bio-cell and polymer film via AFM(Atomic Force Microscopy) modulation and Force curve mode image.

김창호, \*차호석

ANT Co. 연구지원팀 \*ANT Co. Technical Sales

우리는 bio cell 과 polymer 박막의 stiffness 의 물리적 성질을 AFM(Atomic Force Microscopy) modulation mode 와 Force curve mode image 를 통하여 측정하였다. fixed bio-cell 세포막의 세포질과 세포핵에서의 stiffness 를 측정하여 특성을 연구하여 drug delivery 에 대한 기반 연구를 수행하였고 또한 polymer bead 와 같이 인규베이션된 fixed cell 에 대한 AFM stiffness 를 측정하여 세포막에서의 polymer bead 의 탐지 가능성을 확인하려고 하였다. 또한 polymer 박막에 대한 stiffness 이미지를 측정하여 polymer 박막의 국부적인 물리적 특성을 확인하였고 copolymer 에 대한 국부적인 polymer 의 분산 정도를 확인하는 실험을 수행하였다.

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## Further Investigation of Preparation of Polyynes by Laser Ablation of Graphite in Liquid Phase

신승근, 송재규, 박영은, 박승민

경희대 화학과

Polyynes were formed by laser ablation of a graphite target at 1064 nm and identified by analyzing UV absorption spectra in deionized water, various aqueous solutions and solvents (D<sub>2</sub>O, n-hexane, c-hexane, acetonitrile). We investigated that the major UV absorption peaks coincide with the electronic transitions corresponding to linear polyynes chain (C<sub>n</sub>H<sub>2</sub>; n = 6, 8, 10). The peak intensities increased when polyynes were produced by irradiating the target immersed in acidic media, while those were relatively weak in basic media. This leads us to conclude that OH<sup>-</sup> or H<sup>+</sup> ions play an important role in the formation of polyynes. With increase of the temperature (275K, 283K, 303K, 313K), the effects of keeping time on the UV absorption peak intensities of a polyyne solution decrease also. We obtained that absorption spectra of polyynes obtained by laser ablation of graphite target at different fractions of volumes (H<sub>2</sub>O:D<sub>2</sub>O).

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## Recombinant Production and NMR Structural Studies of Transmembrane Domain of Syndecan-4

최성섭, 박태준, 김지선, 박유근, 김용애

한국의국어대 화학과

The transmembrane heparan sulfate proteoglycan, syndecan-4, plays potentially important roles that may influence tissue development and repair, as well as the pathogenesis of numerous diseases. Recently, a number of studies have been conducted on the structural properties and biological functions of the syndecan-4 cytoplasmic domain or extracellular domain. However, previous attempts to understand the structure and function of the syndecan-4 transmembrane domain (Syd4-TM) have been marred by experimental adversities due to insufficient yields and low solubility. To investigate the structural and functional properties of Syd4-TM, an efficient method of preparing milligram quantities of the corresponding peptide is necessary. Herein, we present an efficient method for the recombinant expression and purification of Syd4-TM peptide. The fusion protein was expressed in the form of inclusion bodies. Syd4-TM peptide was released from the fusion protein by cyanogen bromide cleavage, and then purified by semi-preparative reversed-phase high performance liquid chromatography. Finally, more than 5 mg of Syd4-TM peptide was obtained with high purity from one liter of M9 minimal media under optimized conditions. The peptides were identified by polyacrylamide gel electrophoresis and mass spectrometry. The preliminary biophysical properties of recombinant Syd4-TM peptide were studied by circular dichroism (CD) and nuclear magnetic resonance (NMR) spectroscopy. The analysis of the CD spectrum shows that Syd4-TM adopts a stable  $\alpha$ -helical structure in micelle environment. And solution NMR studies showed that Syd4-TM forms an asymmetric dimer in the DPC and SDS micelles.

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발표분야: 물리화학

발표종류: 포스터, 발표일시: 목 10:30~12:30

## Fluorescence Properties of Catechin in Aqueous Solution

박형련, 염지은, 양익준, 양정임, \*윤진아, \*\*박기민

전남대 화학과 \*경상대 교육대학원 교육학과 화학교육전공 \*\*경상대 화학교육과

Green tea is one of the most widely used beverages in the world, because there are high content of polyphenols which act as antioxidant function. Catechin (5,7,3',4'-tetrahydroxyflavan-3-ol) is also a polyphenolic substance and gives beneficial effects on human health. It is therefore studied on the fluorescence properties of catechin in aqueous solution. The substance is absorbed below the light of 300 nm in the deaerated water. As the time passes, catechin is oxidized in aqueous solution and new peaks were appeared above the wavelength of 300 nm. The result is similar to the case of basic solutions. The substance emits weak fluorescence. The fluorescence maximum peaks are obtained about at 320 nm, 475nm. Its fluorescence spectra is also changed according to the pH values as well as the storage time in the solution. As the time passes after catechin dissolves in aqueous solution, the fluorescence maximum peak at 320 nm is disappeared.



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장소: 제주ICC

발표코드: I-PHYS.P-76

발표분야: 물리화학

발표종류: 포스터, 발표일시: 목 10:30~12:30

## Spectroscopic Properties of Quercetin and Apigenin in Hydro-organic Mixed Solvents

박형련, 염지은, 양익준, 양정임, \*윤진아, \*\*박기민

전남대 화학과 \*경상대 교육대학원 교육학과 화학교육전공 \*\*경상대 화학교육과

The fluorescence properties of quercetin(QCT) and apigenin(API) were studied in CH<sub>3</sub>OH-H<sub>2</sub>O and CH<sub>3</sub>CN-H<sub>2</sub>O mixed solvents. Compared with the molecular structure of QCT, API doesn't have the -OH group at 3-carbon and 3'-carbon. Without this difference, the molecular structure of QCT and API is the same. Due to the -OH at 3-carbon, the Brings of QCT deviate slightly from the plane of A and C rings but the B ring of API will become coplanar with the A and C ring. The UV/visible absorption spectra of QCT and API are similar to each other but the fluorescence properties of two molecules are quite different. In QCT, the only S<sub>2</sub>→S<sub>0</sub> emission is observed when the molecule is excited to the S<sub>2</sub> state. In API, if molecule is excited to S<sub>2</sub> state, the only S<sub>2</sub>→S<sub>0</sub> emission is shown but the molecule is pumped to S<sub>1</sub> state, S<sub>1</sub>→S<sub>0</sub> emission is also exhibited with the similar intensity. All of the emission bands of QCT and API are broad and the intensity decreases quickly as the H<sub>2</sub>O composition in the solvent increases. When the amount of H<sub>2</sub>O exceeds 50%, all of the fluorescence emission disappears. The fluorescence center of gravity, fluorescence quantum yield and fluorescence lifetime are measured to investigate the properties of QCT and API.

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발표코드: I-PHYS.P-77

발표분야: 물리화학

발표종류: 포스터, 발표일시: 목 10:30~12:30

## Comparison between Time-dependent Wavepacket Propagation and Ab Initio Molecular Dynamics Methods

안희선, 백경구

강릉대 화학과

Time-dependent Wavepacket propagation (TDWP) 방법은 Quantum Effects 를 잘 다루는 장점을 가지지만, 3 차원보다 더 큰 자유도로 확장하기 어렵다. 반면에 Ab Initio Molecular Dynamics (AIMD) 방법은 보다 일반적인 다-원자 분자들의 다-차원을 다룰 수는 있지만 양자효과를 충실하게 포함시키기 어렵다. 본 연구에서는 먼저 전자 상태들 사이의 비-단열 (Non-adiabatic) 효과가 크게 나타나는 3-원자 및 4-원자로 구성된 작은 분자들의 저-준위 전자상태들의 Potential Energy Surface (PES)와 비-단열 짝지음 (Non-adiabatic coupling) 항을 구성하는 방법들을 비교 분석하였다. 그리고, 이들을 사용하여 대략 수백 펨토-초까지의 광-동력학 초기 과정들에 대하여 TDWP 방법과 AIMD 방법을 동시에 적용한 후, 그 결과들을 비교 분석하여 AIMD 방법에서 양자효과를 보다 충실하게 고려하는 방안을 탐색하였다.

일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: I-PHYS.P-78

발표분야: 물리화학

발표종류: 포스터, 발표일시: 목 10:30~12:30

## Catalytic Activity of Pt/CNT for Complete Decomposition of Volatile Organic Compounds

오준식, 정광우

원광대 화학과

Catalytic oxidation is an attractive way to destroy trace quantities of volatile organic hazardous pollutants in air. In this study, the catalytic decomposition of volatile organic compounds (VOCs) was investigated using a flow-type Pt/CNT (carbon-nanotube supported Pt nano-particles) catalysis reactor at the temperature below 200 °C. The catalyst was characterized by its unique hydrophobic property which facilitates the conversion of target compounds with high activity at relatively low temperatures unaffected by water vapor concentrations in the system. The surface composition and morphology of Pt/CNT catalyst were analyzed by EDS, XPS, SEM, TEM, and XRD. The influence of sample concentration and the reactor temperature as well as the surface kinetic mechanism for the catalytic reaction will also be discussed. Primitive results suggest that Pt/CNT catalytic system will be capable of use in a wide range of applications, particularly for in-situ detoxification of hazardous compounds in air.

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장소: 제주ICC

발표코드: I-PHYS.P-79

발표분야: 물리화학

발표종류: 포스터, 발표일시: 목 10:30~12:30

## **Cobalt and Cobalt Oxide Nanoparticles Produced by Pulsed Laser Ablation in Various Solvents**

정현진, 안아름, 문철주, 최명룡

경상대 화학과

The formation of cobalt nanoparticles by pulsed laser ablation of cobalt plate in various solvents is reported. A pulsed Nd:YAG laser (1064 nm, 10 Hz, 7 ns) is used to produce the cobalt and cobalt oxide nanoparticles, of which size and composition dependence is demonstrated by the laser fluence, ablation time, and the nature of the liquid.

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장소: 제주ICC

발표코드: I -PHYS.P-80

발표분야: 물리화학

발표종류: 포스터, 발표일시: 목 10:30~12:30

## Catalytic Dechlorination of m-dichlorobenzene (m-DCB) using Pd/Mg Nanoparticles Produced by Pulsed Laser Ablation(PLA)

안아름, 정현진, 문철주, 최명룡

경상대 화학과

Chlorinated organic compounds are widely used in the chemical and electronic industries. Disposal of chlorinated organic wastes in such a way as to minimize the environmental hazards has become an urgent issue nowadays. Many efforts for reducing the environmental hazards have promoted to develop a variety of methods for the dechlorination of chlorobenzene compounds. Accompanying such efforts, in this study, we have prepared Mg nanoparticles using an Mg plate via liquid phase - pulsed laser ablation (LP-PLA). The nanoparticles were later palladized, making Mg/Pd bimetallic nanoparticles by redox reactions, and played as a catalyst for the dechlorination of m-dichlorobenzene (m-DCB).

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장소: 제주ICC

발표코드: I-PHYS.P-81

발표분야: 물리화학

발표종류: 포스터, 발표일시: 목 10:30~12:30

## Insight of dominating factors for the stability of bio-nanostructures

박성병, 이명수, 신석민

서울대 화학부

Interests in artificial bio-nanostructures, including peptide-based self-assembled nanostructures, have been very intense. Recently, Myongsoo Lee et. al. synthesized polymers of beta-sheet-forming peptide (WKWEYWKWEW) with the hydrophilic oligoether dendron (T3). It was found that the most stable structure for the peptide T3 aggregates is a nanoring structure with highly uniform diameter. Other analogous T-shaped peptides with different relative volume fraction of a dendron to a beta-sheet peptide were found to form aggregate structures other than nanoring formation. We performed MD simulations on the self-assembled structures of the peptide T3 and other analogous peptides using all-atom AMBER force field 96 under the implicit solvation condition. For the peptide without the bulky dendron (T1), bilayer structures of anti-parallel beta-sheet are found to be stable. And we examined the stability of various sizes of nanoring structures for T3. Nanorings with ca. 40 monomers of T3 are found to be stable. Over the simulation time the diameter for the inner pore sustains in 3.5–4.5 nm, but the whole structure has ca. 11 nm of the diameter and ca. 4 nm thickness, which is consistent with the experimental observations, ca. 11 nm diameter and ca. 3 nm thickness. Analyses for the simulation results suggest that important factors determining the self-assembled structures include H-bonding between backbones of monomers, the electrostatic interactions between Lys and Glu residues, and the alignments of bulky TRPs. Understanding the basic driving force for the formation of such peptide-based self-assembled nanostructures is expected to be useful in designing noble functional bio-nanostructures.

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장소: 제주ICC

발표코드: I-PHYS.P-82

발표분야: 물리화학

발표종류: 포스터, 발표일시: 목 10:30~12:30

## Effect of glass texture for efficiency improvement of dye-sensitized solar cells

남상훈, 부진효

성균관대 화학과

The etching of glasses in aqueous hydrofluoric acid (HF) solutions is applied in many technological fields. In this study, we fabricated textured glass surface using HF (49%)/DI water solution for improvement of current density in dye-sensitized solar cells. The textured glass had higher surface roughness than bare glass by atomic force spectroscopy (AFM). Also, it had high transmittance about 80%. Therefore, current density was about 20% increasing by textured glass. This means that increased the electron lifetime for light trapping effect. The process could be applicable in texturing glass surface to fabricate solar cell in industrial scale.

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장소: 제주ICC

발표코드: I-PHYS.P-83

발표분야: 물리화학

발표종류: 포스터, 발표일시: 목 10:30~12:30

## Simultaneous Observation of Lipid Mixing and Content Release in SNARE-mediated Intracellular Membrane Fusion

최윤미, 정지원, \*이남기, 김성근

서울대 화학부 \*포항공과대 시스템생명공학부/물리학

Membrane fusion in cells is of vital importance in numerous biological processes, including neurotransmitter release through synaptic membrane fusion mediated by soluble N-ethylmaleimide-sensitive factor attachment protein receptors (SNAREs). As a model system for intracellular membrane fusion, we employed SNARE-containing vesicles labeled with DiO and DiI and carried out FRET experiments for lipid mixing as well as content release at the single vesicle level. By utilizing the capability of 3-color alternating-laser excitation FRET to simultaneously detect inter-probe distance and stoichiometry, we demonstrated the content mixing of vesicles when Cy5/quencher dual-labeled molecular beacon encapsulated in a vesicle encounters its complementary DNA in the other vesicle.



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발표코드: I -PHYS.P-84

발표분야: 물리화학

발표종류: 포스터, 발표일시: 목 10:30~12:30

## **Temperature-dependent Total Internal Reflection Fluorescence Study of Real-time Enzymatic Reaction Dynamics of 10-23 Deoxyribozyme**

정지원, 김성근

서울대 화학부

Deoxyribozyme is a family of DNA with enzymatic functions such as RNA-cleaving activity carried by one of its members, 10-23 deoxyribozyme. In an attempt to observe such enzymatic action in real time, we employed total internal reflection fluorescence (TIRF) to track individual steps of the reaction between 10-23 deoxyribozyme and its target RNA. In particular, we carried out temperature-dependent TIRF experiments to elucidate the chemical kinetic aspects of these reaction steps.

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장소: 제주ICC

발표코드: I-PHYS.P-85

발표분야: 물리화학

발표종류: 포스터, 발표일시: 목 10:30~12:30

## Fluorescent Nanodiamond Biomarker for Targeted Binding in HeLa Cell

이종우, \*이선주, \*이연, \*김성근

서울대 생물물리 및 화학생물학과 \*서울대 화학부

Fluorescent nanodiamond (FND) is much superior to quantum dots or organic dyes as a biomarker since it is nontoxic and highly photo-stable. Because a long-time measurement is possible, FNDs can be a bio-tracker as well. There exists a huge obstacle, however, with the in vivo use of FNDs since they tend to strongly aggregate at physiological salt concentrations. In order to prevent such aggregation and make FNDs suitable for in vivo applications, we subjected FND particles to a diverse range of surface treatments and found that their aggregation is highly reduced. By cross linking antibodies, we also observed the binding of FND particles to a specific region in a HeLa cell.

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발표코드: I-PHYS.P-86

발표분야: 물리화학

발표종류: 포스터, 발표일시: 목 10:30~12:30

## Expansion Cooling in the Matrix Plume is Under-Recognized in MALDI Mass Spectrometry

배용진, \*문정희, 김명수

서울대 화학부 \*한국생명공학연구원 단백질의학연구센터

Time-of-flight (TOF) mass spectra for a peptide ( $Y_6$ ) were obtained by utilizing matrix-assisted infrared laser desorption ionization (IR-MALDI) with glycerol as matrix and by utilizing ultraviolet MALDI with  $\alpha$ -cyano-4-hydroxycinnamic acid (CHCA), sinapinic acid (SA), and 2,5-dihydroxybenzoic acid (DHB). Collisional activation during ion extraction and exothermicity in gas-phase proton transfer were found to be unimportant as the driving forces for in-source (ISD) and post-source (PSD) decays, indicating that the thermal energy acquired during photo-ablation is responsible for their occurrence. The temperatures of  $[Y_6 + H]^+$  in 'early' and 'late' matrix plumes were estimated by kinetic analysis of ISD and PSD yields, respectively. Their order was glycerol < DHB  $\approx$  SA < CHCA in early plume and glycerol < DHB < SA < CHCA in late plume. For each matrix, the temperature in late plume was lower than in early plume by 300-400 K, which was attributed to expansion cooling. The model (thermalization followed by expansion cooling) proposed to explain the occurrence of both rapid ISD and slow PSD is not only in sharp contrast with but also mutually exclusive with the prevailing explanation that the exothermicity in proton transfer and in-plume collisional activation are the driving forces for ion fragmentation in MALDI. The model also explains why MALDI is more successful for mass spectrometry of labile molecules than other desorption techniques that do not utilize matrix. Factors affecting plume temperature are also discussed.

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발표코드: I-PHYS.P-87

발표분야: 물리화학

발표종류: 포스터, 발표일시: 목 10:30~12:30

## Self-Assembled Monolayers of Pyrrole-Terminated Alkanethiols on Au(111)

이동진, 신동근, 강훈구, \*Eisuke Ito, \*\*Masahiko Hara, 한진욱, 노재근

한양대 화학과 \*RIKEN \*\*RIKEN, TITech

Self-assembled monolayers (SAMs) of alkanethiols on gold are key elements for building many systems and devices with applications in the wide field of nanotechnology. Pyrrole-terminated SAMs were formed by the spontaneous adsorption of 6-(*N*-pyrrolyl)hexane-1-thiol, 8-(*N*-pyrrolyl)octane-1-thiol, 10-(*N*-pyrrolyl)decane-1-thiol, and 12-(*N*-pyrrolyl)dodecane-1-thiol 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 thermal desorption spectroscopy (TDS). STM observation shows that the SAMs formed in solution have mainly disordered domains, but the SAMs formed by vapor deposition have more uniform surface with clear vacancy islands. XPS measurements for pyrrole-terminated alkanethiols SAMs show that sulfur atoms are chemically bond to the gold surface. In addition, TDS measurements reveal that the SAMs were mainly desorbed as decomposed species after dissociative reaction of C-S bond during heating.

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발표코드: I-PHYS.P-88

발표분야: 물리화학

발표종류: 포스터, 발표일시: 목 10:30~12:30

## Unique Ordered Domains of Biphenylthiol Self-Assembled Monolayers on Au(111)

강훈구, \*Eisuke Ito, \*\*Masahiko Hara, 노재근

한양대 화학과 \*RIKEN, Japan \*\*TITech, Japan

Biphenylthiol (BPT) 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 biphenylthiol (BPT) self-assembled monolayers (SAMs) on Au(111) were examined using scanning tunneling microscopy (STM) and X-ray photoelectron microscopy (XPS). STM imaging revealed that the structural order of BPT SAMs formed in a 0.01mM ethanol solution at 60 °C decreases with increasing immersion time. Interestingly, BPT SAMs formed after 30 min have unique ordered domains containing well-ordered ( $3 \times 3$ ) R30° structures and bright rows that are connected by small aggregated domains with a periodicity of approximately 10 Å, results that have never been observed for other thiol SAM systems. Distances between the bright rows were 20–35 Å. The bright small domains contained five or six BPT molecules each, which may have originated from differences in the adsorption orientations of biphenyl groups that were induced by localized interactions between them. XPS measurements for BPT 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 BPT SAMs on gold surfaces.

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발표코드: I-PHYS.P-89

발표분야: 물리화학

발표종류: 포스터, 발표일시: 목 10:30~12:30

## Formation and Characterization of Alkanethiol Self-Assembled Monolayers on GaAs Surface

서한민, 강훈구, \*Eisuke Ito, \*\*Masahiko Hara, 노재근

한양대 화학과 \*RIKEN, Japan \*\*TITech, Japan

The formation and thermal stability of alkanethiol ( $\text{CH}_3(\text{CH}_2)_n\text{SH}$ ,  $n=7, 11, \text{ and } 17$ ) self-assembled monolayers on n-type GaAs(001) has been systematically studied by atomic force microscopy (AFM), X-ray photoelectron spectroscopy (XPS), thermal desorption spectroscopy (TDS), contact angle (CA) measurements. It was found that the formation of alkanethiols SAMs was significantly influenced by alkyl chain length, solution temperature, and immersion time. The CAs for octanethiol, dodecanethiol, and octadecanethiol SAMs were measured to be  $93^\circ$ ,  $97^\circ$ , and  $106^\circ$ , respectively, which means that alkanethiols with a longer alkyl chain generates high-quality SAMs. We observed strong XPS peak in the S 2p region at 162 eV, which implies the formation of chemisorbed ODT SAMs on GaAs. In addition, desorption peaks corresponding  $\text{CH}_3(\text{CH}_2)_{17}\text{S}^+$  species from ODT SAMs on Au(111) and GaAs surfaces were observed at 170 and 240  $^\circ\text{C}$ , respectively, which means that ODT SAMs on GaAs have a higher thermal stability compared to those on Au(111).

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발표코드: I-PHYS.P-90

발표분야: 물리화학

발표종류: 포스터, 발표일시: 목 10:30~12:30

## Fabrication of Thiol-Terminated Self-Assembled Monolayers Using Acetyl-Protected Alkanedithiols on Au(111)

구경빈, 강훈구, 신승훈, \*Eisuke Ito, \*\*Masahiko Hara, 노재근

한양대 화학과 \*RIKEN, Japan \*\*TITech, Japan

Alkanedithiol self-assembled monolayers (SAMs) on gold have attracted much attention because of the possibility of using them as linkers between two metals for molecular electronic applications. However, it has been generally believed that dithiols are difficult to form well-ordered SAMs with free SH end-groups. One of main problems is related to the formation of striped phase with the two thiol groups bound to the gold surface. Therefore, to overcome this problem, we synthesized a molecule containing a active SH group and an acetyl-protected SH group as the end groups, thioacetic acid S-(8-mercaptooctyl)ester (TMOE). To compare the formation of TMOE SAMs, we also used 1,8-octanedithiol (ODT) and S-(8-acetylsulfanyl-octyl)ester (TASOE). The surface structure, binding condition, and thermal desorption behavior of these SAMs on Au(111) were characterized using scanning tunneling microscopy (STM), X-ray photoelectron spectroscopy(XPS), and thermal desorption spectroscopy (TDS). We found that the adsorption of TMOE molecules creates uniform SAMs with thiol-terminated surface compared to ODT and TASOE.

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장소: 제주ICC

발표코드: I-PHYS.P-91

발표분야: 물리화학

발표종류: 포스터, 발표일시: 목 10:30~12:30

## Efficient Ground-state Depletion Microscopy Using Photo-switchable Dyes

권지웅, \*황지희, \*\*김성근

서울대 생물물리 및 화학생물학과 \*서울대 생물물리 및 화학생물학 \*\*서울대 화학부

By using particular photophysical properties of some photo-switchable dyes, we explored more efficient ways to observe small molecules in biological structures by ground-state depletion (GSD) microscopy. In typical GSD microscopy, it takes about several minutes to acquire an image due to the time delay between imaging points, which is limited by the time it takes to return to the singlet ground ( $S_0$ ) state. This time delay can be greatly reduced if a stimulus can be employed to induce the transition for the dye molecule from a triplet (or other excited) state to the  $S_0$  state. By adopting photo-switchable dyes in GSD microscopy, we were able to obtain sub-diffraction limit optical images at a much faster imaging rate than in conventional GSD microscopy.



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발표코드: I-PHYS.P-92

발표분야: 물리화학

발표종류: 포스터, 발표일시: 목 10:30~12:30

## Synthesis of Metallic $\text{ReO}_3$ Nanowires

명동신, \*이유민, 이재연, \*\*김명화

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Rhenium trioxide ( $\text{ReO}_3$ ) is well known as an unusual transition metal oxide with unexpectedly high electrical conductivity close to that of copper. We present the synthesis of highly crystalline metallic rhenium trioxide ( $\text{ReO}_3$ ) nanowires.  $\text{ReO}_3$  nanowires were grown on a 200 nm silica-covered Si (001) wafer by atmospheric-pressure chemical vapor deposition (APCVD) at about 300 °C without any catalyst. The wafer was placed in the quartz boat approximately 15 cm downstream from the fine mashed  $\text{ReO}_3$  powder and heated at 320 °C with flowing of high purity Ar (500 sccm) for 2 h and then kept at 450 °C for an additional 3 h. The two-step heating enhanced the growth of  $\text{ReO}_3$  nanowires. The structures and morphologies were examined using scanning electron microscopy (FE-SEM) and high-resolution electron microscopy (HRTEM). Based on HRTEM, the  $\text{ReO}_3$  nanowires exhibit a core of perfect cubic perovskite type single crystal structure with a shell of thin amorphous and disordered structures of less than 2 nm in the near surface layers. Possibly this is due to proton intercalation induced by the surface reaction of single crystal  $\text{ReO}_3$  with water.

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## 2D IR Correlation Analysis of NiPAAm Gelation Process

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Poly(N-isopropylacrylamide) (PNiPAAm) hydrogel is a smart hydrogel, which can be applied to drug delivery, tissue engineering, artificial muscles, etc. PNiPAAm hydrogel has a coil-globule transition above its lower critical solution temperature (LCST, at ~33 °C). The mechanism of chemical cross-linking of PNiPAAm hydrogel has been extensively studied by using, NMR, light scattering, neutron scattering, and IR spectroscopy. However detail of mechanism of NiPAAm gelation process is not clearly understood. In this presentation, we have studied the mechanism of NiPAAm gelation process by using 2D IR correlation spectroscopy. Details of mechanism of NiPAAm gelation process will be discussed. Acknowledgement This work was supported by the BK 21 program from the Ministry of Education, Science and Technology of Korea.

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## Crystallization of spin-coated films of P(HB-co-HHx)/PEG blends

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Poly(3-hydroxybutyrate-co-3-hydroxyhexanoate) (P(HB-co-HHx)), which is a new member of the polyhydroxyalkanoate (PHA) family, has been studied extensively. We have recently investigated thermal behavior of spin-coated films of PHB-co-HHx copolymer. It is also important to investigate the thermal behavior of P(HB-co-HHx) in the presence of other polymers like poly(ethylene glycol) (PEG). P(HB-co-HHx) is fully miscible with poly(ethylene glycol) (PEG). In this study, to investigate crystallization of spin-coated films of P(HB-co-HHx)/PEG blends, P(HB-co-HHx) blends with a PEG content of 2, 10, 20 wt% were prepared from chloroform solution. Crystallization of spin-coated films of P(HB-co-HHx)/PEG blends are investigated by 2D correlation spectroscopy. The details of 2D correlation spectra of P(HB-co-HHx)/PEG blends will be discussed.

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## Effect of $\gamma$ -butyrolactone as additive to UV curing resin polymer gel electrolytes for a dye-sensitized solar cell

박근우, 정영미, \*정재원, \*\*황철균

강원대 화학과 \*한국이엔에쓰(주) \*\*나노융합실용화센터 나노융합개발팀

The development of renewable energy sources for future energy systems, especially solar energy, has been growing at an ever increasing pace due to global warming and limited availability of fossil fuels. The dye-sensitized solar cell (DSSC) provides an attractive alternative to solid-state photovoltaics for the conversion of solar energy to electricity. Especially it has a great potential of low cost compared to conventional silicon-based solar cells. DSSC based on  $\text{TiO}_2$  as the nanostructured electrode are capable of achieving efficiencies of 11%. The high efficiency, however, can be obtained only when employing volatile electrolytes, which commonly have some restrictions in guaranteeing stability. For the practical application of DSSC, electrolytes with reliable stability, as well as high efficiency, are highly demanded. In this study, we studied the effect of  $\gamma$ -butyrolactone as additive to UV curing resin gel polymer electrolytes. UV curing resin gel polymer electrolytes were prepared by varying the concentration of additive. The photovoltaic performance of UV curing resin polymer gel electrolytes based DSSC will be discussed.

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## **SERS Based Selective Bioseparation**

홍원진, \*Lei Chen, 이영주, \*Bing Zhao, 정영미

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As an ultrasensitive technique, surface-enhanced Raman scattering (SERS) has been proven to have great potential in high throughput protein detections. Magnetic nanoparticles have been used as a separation tool combined with SERS for detection of biomaterials. For protein detection, magnetic nanoparticles coated with Ag or Au have been introduced. In this study,  $\text{Fe}_3\text{O}_4/\text{SiO}_2/\text{Au}$  core/shell nanoparticles were synthesized by deposition of Au on the preformed  $\text{Fe}_3\text{O}_4/\text{SiO}_2$  nanoparticles for protein separation. The products were characterized by means of SEM, TEM, and VSM. Details of SERS with core/shell nanoparticles will be discussed.

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## Vibrational Optical Activity Study for Protein Denaturation

유수련, 강대훈, \*B. Czarnik-Matusiewicz, \*\*Rina K. Dukor, \*\*\*Laurence Nafie, 정영미

강원대 화학과 \*University of Wroclaw, Poland \*\*BioTools Inc., U.S.A. \*\*\*BioTools Inc. U.S.A. Syracuse University, U.S.A.

Vibrational optical activity (VOA) spectroscopy is widely used for conformational studies of chiral molecules. Vibrational circular dichroism (VCD) spectroscopy measures the differential absorbance of left and right circularly polarized light in the infrared region originating from molecular vibrations. Raman optical activity (ROA) measures a small difference in the intensity of Raman scattering from chiral molecules in right and left circularly polarized incident laser light. VCD and ROA both are a relatively new technique for the study of conformational preference of proteins and peptides. Two-dimensional (2D) correlation spectroscopy has attracted a high level of interest of analytical science community, as it provides considerable utility and benefit in many fields of spectroscopic studies. In this study, we have applied 2D correlation spectroscopy to VCD and ROA spectra of the pH-dependent bovine  $\alpha$ -lactalbumin to investigate the molten globule state. The details of molten globule state of bovine  $\alpha$ -lactalbumin will be discussed. It is a key issue to understand bases of the secondary structure changes that are responsible for various conformational diseases.

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## High-yield synthesis of silver nanoplates in aqueous solution

LIU ZHUN, ZHOU HU, PIAO LONGHAI, 김상호

공주대 화학과

Silver nanoplates were synthesized in high yield through the modified polyol reduction method where medium molecular weight poly (ethylene glycol) was used as a reducing agent. The UV-visible spectra of the nanoplate suspensions display an intense in-plane dipolar Plasmon resonance band, as well as weak bands for in-plane and out-of-plane quadrupolar resonances. The SEM images show that the silver nanoplates have the thickness of ~20nm and the diameter of >100nm. Further study suggests that the larger nanoplates were formed by self-assembly of those of smaller ones due to the strong dipole-dipole interaction between adjacent nanoplates. These nanostructures of silver with unique planar shapes have many applications in areas of photonics, optoelectronics and optical sensing.

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## Molecular Structures and Electronic Spectra of Methyl Pyropheophorbide-a Pyrazol Derivatives: a Density Functional Theory

최상준

인제대 의생명화학과

광역학치료(PDT)는 광민감성물을 주사하고 가시광선으로 광민감성 물질을 활성화하여 생성된 초과산화물(Superoxide,  $O_2O^{\cdot -}$ , 단일항산소(Singlet Oxide), 삼중항산소(Triplet Oxide), 라디칼산소(Radical Oxygen)에 의해 암세포를 파괴하는 기술이다. 최근 새로합성된 피라졸을 포함하는 Methyl Pyropheophorbide-a 유도체인 3-[3-5-methyl-H-pyrazol-4-yl]-3-devinyl-pyropheophorbide-a methyl ester(HPMPPa)와 3-[3,5-methyl-1-phenyl-pyrazol-4-yl) methyl]-3-devinyl-pyropheophorbide-a methyl ester (PPMPPa)의 구조와 Spectra 를 연구하였다. 이들 물질은 피라졸의 생물학적특성인 항암성, 항균성, 항바아러스성과 Chlorin macrocycle 의 PDT 특성 둘다를 가진다고 알려져있다. 또한 피라졸기에 HPMPPa(피라졸기에 치환체가 없는 화합물)가 PPMPPa(피라졸기에 친유성 방향족고리가 결합된 화합물)보다 암세포에 대한 생물학적 약효가 뛰어나다고 알려져 있다. 하지만 PDT 의 흡수파장(Q)은 둘다 661 nm 이다. 크로린(chlorin) system 위에 피라졸 치환체가 화학적관점에서 UV-Visible 파장에 영향을 줄 것인지 여부를 알아 보고, 주지않는다면 왜 주지않는가를 구조적관점 분광학적인 관점에 연구한 결과 구조적관점에서는 HPMPPa 와 PPMPPa 의 Chlorin macrocycle 의 구조가 매우 같으며, 분광학적 관점에서도 전자 밴드성질(electronic band character, Q)이 657nm 와 658nm 로 매우유사하였다. 이는 실험값 661nm 와 잘일치한다. 이결과는 HPMPPa 와 PPMPPa 분자의  $\pi \rightarrow \pi^*$  전이가 chlorin macrocycle 이 지배적이기 때문이다. 따라서 피라졸은 PDT 파장에 영향을 주지 않음을 알았다. 계산 방법은 구조연구는 M06-2X/6-311+G(d,p) 함수를 사용했고, 분광학적 계산은 TDM06-2X 를 사용하고 basis set 는 6-31+G(d,p)와 6-311+G(d,p)를 사용하였다.



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## Growth temperature and contact resistance of gold/pentacene

김윤복, 전동렬

서울대 물리교육과

The properties of metal/organic interface are very different from those of metal/inorganic interface because of intermixing at the interface and the dipole layer. The degree of intermixing depends on the growth condition such as temperature and deposition rate. We have compared the morphology and the contact resistance of Au electrode deposited on pentacene at room and liquid nitrogen temperature. We measured the total resistance as a function of pentacene channel length and estimated the Au/pentacene interface resistance by extrapolating the total resistance to zero channel length. The result showed that both the total and contact resistance of Au electrode deposited at liquid nitrogen temperature was smaller. Atomic force microscopy and scanning electron microscopy revealed that the interface formed at room temperature was much more mixed. The structural deformation of pentacene molecules caused by Au particle penetration seems to create traps rather than creating conductive channels. We performed Fourier transform infrared (FTIR) spectroscopy to check the amount of deterioration of pentacene molecules due to the Au penetration. For both deposition temperatures, the FTIR absorption peak intensity decreased upon Au deposition, but the room temperature deposition resulted in about twice the decrease. Furthermore, the peak position of room temperature deposition sample shifted to a lower wavenumber. This indicates that the pentacene crystalline structure at the contact was damaged more by room temperature deposition due to higher Au diffusion and penetration, which results in higher Au/pentacene contact resistance. We will also discuss X-ray photoemission spectroscopy results.

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## Designed neutral radicals based on diazaphenalenyl derivatives: spin sources for controlled intramolecular magnetic interactions

고정철, 문종훈, 손성욱, 이진용

성균관대 화학과

We designed the novel neutral radical series (DP1-6) based on diazaphenalenyl by adding oxygen atoms in nitrogen site. As spin sources in diradical system, designed radicals were newly investigated. And we evaluated the magnetic coupling constants of designed radicals and famous neutral radicals as references in specially designed diradical systems (1st system) by DFT method. The magnetic interactions are shown in order of  $DP3 > DP4 > DP2 > DP6 > DP5 > DP1$ . Especially, DP3 have the stronger magnetic interactions than well-known radicals (IN, and o-VER(C)). The trend of magnetic interactions was fully understood by spin density distributions and NICS values. The heteroatomic modulations in diazaphenalenyl provoked the controlled intramolecular magnetic interaction in diradical system. And another two diradical systems (2nd and 3rd systems) which have planar geometries and same bond distances reproduced the same tendencies of magnetic interactions. Therefore, we proposed that designed radicals applicable to control the intramolecular magnetic interactions of organic magnets. At last, we investigated the HOMO-LUMO energy gap of 2nd diradical system to measure the radical stabilities. These results will be helpful in the design and control the organic magnetic materials incorporated with diazaphenalenyl derivatives.

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## Theoretical Investigations on Charge Transport Properties of Stacked Annelated $\beta$ -Trithiophenes

Liu Hongguang, 이진용

성균관대 화학과

Density functional theory (DFT) calculations were performed using a MPWB1K function to interpret the charge transport (CT) properties of stacked annelated  $\beta$ -trithiophenes molecules. The goal was to help understand how the chemical composition, face-to-face stacking, intra- and intermolecular correlations and the applied electric field affect the CT properties of this organic semiconductor compared to those of the edge-to-face “herringbone” motif. The variations in the frontier orbitals, energy gap, nonadiabatic electron attachment energies (EAE) and vertical detachment energies (VDE) were investigated under an external electric field as a function of the number of stacked layers ( $n$ ). Two possible CT pathways, monomer-to-monomer (MM) and dimer-to-dimer (DD) transports, were postulated to determine the charge carrier conductivities of these molecules. The results highlight that the intermolecular electronic couplings and electrostatic interactions can significantly affect the stacking geometry even in more extended structures; displaced stacks with smaller interlayer spacings resulted in more compact stacking and thus higher CT efficiency; face-to-face stacking geometries can help to reduce the energy gap and VDE. Despite the fact that common thiophene-based oligomers adopting edge-to-face herringbone motifs exhibit p-type (hole-transporting) characters, the face-to-face stacked models based on annelated  $\beta$ -trithiophenes exhibited remarkably increased n-type (electron-transporting) performances.

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## Solvent Effect on the Excited-State Proton Transfer of 7-Hydroxyquinoline Hydrogen-Bonded with Ethanol Dimer

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성균관대 화학과 \*서울대 화학부

Proton transfer from one atom to another is a fundamentally important process that plays a crucial role in lots of reactions. Aromatic molecular complexes involving small polar molecules that can donate or accept a proton are quite attractive model systems. Solvent effect on structures and potential energy surfaces along proton transfer has been studied both in the ground and the excited states of 7-hydroxyquinoline (7-HQ) associating with an ethanol dimer using ab initio calculations. The proton transfer is forbidden in the ground state not only in vacuum but also in solvents. In the excited state, although the proton transfer is still forbidden in vacuum, it is possible to occur in solvents due to greatly reduced barrier (~10 kcal/mol) and more stabilized product. Through frontier orbitals, proton transfer can be enhanced upon excitation. It has also been found from the calculations that the proton-transfer barrier in the excited state decreases as the dielectric constant of a solvent increases due to dipole moment for excited states. Three kinds of solvents are applied to study solvent effect, n-heptane, ethanol, and dimethyl sulfoxide (DMSO). Our calculations are consistent with experimental results that the proton transfer does not take place in the ground state and that the excited-state proton-transfer rate increases as the solvent polarity increases. Our calculated absorption and emission properties are in excellent agreement with experimental results. Projection factors (reflecting geometrical change from the ground state to the excited state) and reorganization energies for several low frequency vibrations in connection with the excited-state proton transfer are discussed as well.

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## Laser-Induced Breakdown Detection: Colloidal property of NOPP 140

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연세대 화학과 \*국민대 생명나노화학과

We have investigated the protein in aqueous solution with the concentration range of ppb by using LIBD (Laser-Induced Breakdown Detection) technique. To determine the colloidal property of protein samples, the exact position of plasma on the laser beam axis is analyzed. It shows that the width of the distribution in plasma events increases as the energy increases in range of 0.28 mJ ~ 0.4 mJ and the minimum detection concentrations decrease as the energy becomes larger. For the samples of  $\alpha$ -lactalbumin and albumin from egg, the distributions of plasma events are fitted to a single Gaussian curve indicating the monomodal colloid property. On the other hand, the sample of urease displays a complicated Gaussian shape, which demonstrates the characteristic of urease existing as a trimer or hexamer in solution. This method was applied to obtain the colloidal property of atypical protein, such as an intrinsically disordered protein (IDP), Nopp140. The results show the dependency on the time needed for the increase in the breakdown probability, indicating the aggregation characteristics of Nopp140 at the initial time stage and then a single Gaussian distribution of plasma events when samples are disaggregated by the sonication. For further understanding of the actual structure of Nopp 140 existing in aqueous solution, comparisons in the plasma distribution with globular proteins are also investigated.

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## **Polyhedral Bimetallic Alloy Nanocrystals Exclusively Bound by {110} Facets: Au-Pd Rhombic Dodecahedron**

이영욱, 한상우

KAIST 화학과

The Au-Pd alloy nanocrystals with an unprecedented rhombic dodecahedral structure, enclosed exclusively by 12 {110} facets, have been prepared in high-yield by a simple one-pot aqueous synthesis method. Successful synthesis of this unique structure bound by high-energy facets was achieved through the kinetically-controlled nucleation and growth process. The rhombic dodecahedral nanocrystals exhibit higher surface-enhanced Raman scattering and electrocatalytic activities compared with {111}-faceted nanoparticles. Facile synthesis of Au-Pd rhombic dodecahedron (RD Au-Pd NC) with ascorbic acid as a reducing agent and cetyl trimethylammonium chloride (CTAC) as a capping agent is presented. The synthesized RD Au-Pd NC were characterized by UV-vis spectroscopy, transmission electron microscopy (TEM), scanning electron microscopy (SEM), X-ray diffraction (XRD), and cyclic voltammetry (CV). The electrocatalytic property of RD Au-Pd NC catalyst for EtOH oxidation was investigated by 0.5 M EtOH in 0.1 M KOH aqueous solution, respectively. To investigate optical enhancing properties of the RD Au-Pd NC, adsorption characteristics of 1,4-phenylene diisocyanide (1,4-PDI), 4-aminobenzenethiol (4-ABT), benzenethiol (BT), and rhodamine 6G (R6G) on RD Au-Pd NC were studied by surface-enhanced Raman spectroscopy (SERS).

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## **Fabrication of Sodium Titanate Nanobelts Electrode on FTO for DSSC**

김태완, 김창우, 강영수

서강대 화학과

The sodium titanate is of particular interest for its wide applications, such as high photocatalytic activities, ion-exchange ability, and photovoltaic characteristics. The sodium titanate nanobelts were synthesized by hydrothermal process in concentrated aqueous NaOH solution. The products obtained from titanium(IV) butoxide was confirmed to be the crystal structure of  $\text{Na}_2\text{Ti}_2\text{O}_4(\text{OH})_2$ . The formation mechanism of the crystal structure in the synthetic process depends on various conditions. Their structure morphology and optical property were investigated with X-Ray Diffraction (XRD), Scanning Electron Microscope (SEM), Transmission Electron Microscope (TEM), and Ultraviolet-visible spectroscopy (UV-Vis). On the basis of their morphology results, sodium titanate nanobelts can be applied for dye sensitized solar cell (DSSC) as working electrode by preparing sodium titanate nanobelts paste on the fluorine-doped tin oxide (FTO) surface by doctor blade technique. Keywords : DSSC, Sodium Titanate Nanobelts, electrode, Hydrothermal method, paste

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## Highly Ordered Mesoporous TiO<sub>2</sub> Electrode with Triblock Copolymer for Dye Sensitized Solar Cell

김창우, 문봉진, 강영수

서강대 화학과

Highly ordered mesoporous TiO<sub>2</sub> film was prepared with triblock copolymer. The mesoporous titania sol was prepared from titanium butoxide and triblock copolymer using sol-gel process. The polymer sol was dropped and spin-coated on the FTO glass with evaporation induced self-assembly method. The mesoporous TiO<sub>2</sub> film on the FTO was obtained after calcination. The geometrical structure is monitored for dye sensitized solar cell. Their morphology was controlled for photoelectrical properties and was characterized for application of dye sensitized solar cell. Mechanisms of formation of the highly ordered meso-structures are proposed and should be very much useful for electrode. Keywords: Mesoporous, Titania, EISA.



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장소: 제주ICC

발표코드: I-PHYS.P-108

발표분야: 물리화학

발표종류: 포스터, 발표일시: 목 10:30~12:30

## Preparation of Highly Ordered Titanium Dioxide Nanotube Arrays by Anodic Oxidation for Dye Sensitized Solar Cell

서상필, 김창우, 강영수

서강대 화학과

Highly ordered titanium dioxide nanotubes were prepared by anodic oxidation of a pure titanium foil in an aqueous solution containing 0.5 to 3.5 wt% fluoride sources. The condition of anodic oxidation was controlled with varying potential and anodizing time. These tubes are well aligned and organized into high-density uniform arrays. While the tops of the tubes are open, the bottoms of the tubes are closed, forming a barrier layer structure similar to that of porous alumina. The average tube diameter, ranging in size from 25 to 65 nm, was found to increase with increasing anodizing voltage, while the length of tube was found to be independent of anodization time. The prepared nanotubes were characterized for application of dye sensitized solar cell. Keywords: TiO<sub>2</sub>, Nanotube, Anodic Oxidation.

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장소: 제주ICC

발표코드: I-PHYS.P-109

발표분야: 물리화학

발표종류: 포스터, 발표일시: 목 10:30~12:30

## Preparation of Cu and Cu<sub>2</sub>O Films with Semi-sphere Shape by Electrodeposition

Zheng jin you, 강영수

서강대 화학과

Uniformed Cu and Cu<sub>2</sub>O films with semi-sphere shape were prepared by the electrodeposition in the Cu(NO<sub>3</sub>)<sub>2</sub> and lactic acid solution. The morphology and crystal structure were characterized by SEM and XRD. The morphology of the films is significantly depending on deposition conditions such as applied potential, pH value and deposition time. As the applied potential increases, the size of Cu particle decreases and Cu film becomes to be more compact. When the potential reached to -0.6 V, the dendrite structure was obtained. The pH change from 1.2 (initial) to 11.2 resulted in the composition change of film from Cu to Cu<sub>2</sub>O. When the electrolyte is acidic, the products are the uniform Cu films. Specially, when the solution was stirred for two weeks, the semi-sphere shape Cu<sub>2</sub>O particle film was appeared. As usually, it is not easy to increase the thickness of Cu<sub>2</sub>O film, but the thickness of the films with semi-sphere shape Cu<sub>2</sub>O particle can get from 2 to 8  $\mu$ m. Keywords: electrodeposition, copper, cuprous oxide

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발표코드: I-PHYS.P-110

발표분야: 물리화학

발표종류: 포스터, 발표일시: 목 10:30~12:30

## Quantum Mechanical Effects on Diffusion Constants and Absorption Spectra in Liquids

김태준, 김효준

동아대 화학과

We study dynamical behaviors and absorption spectra in liquids by evaluating quantum mechanical time correlation functions. We introduce the quantum correction approach to utilize the general relation between quantum and classical correlation functions. In this poster, we investigate diffusion constants of liquid argon and neon, and the absorption spectrum of Nile blue in acetonitrile is also investigated. The quantum diffusion constant of liquid argon is found to be similar to its classical diffusion constant, while non-negligible differences are shown in liquid neon. The higher density liquid shows the bigger difference between classical and quantum diffusion constants. The quantum mechanical effects are clearly shown in absorption spectra.

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장소: 제주ICC

발표코드: I-PHYS.P-111

발표분야: 물리화학

발표종류: 포스터, 발표일시: 목 10:30~12:30

## Imperfect trap effects on diffusion-reaction systems

안서연, 김효준

동아대 화학과

The imperfect trap problems can be easily tackled with the Monte Carlo method that is one of the simplest computer simulations. The analytical results for the imperfect trap problems have also been well-known. However, the relationship between the reaction rate constant in theories and the reaction probability in simulations is ambiguous yet. By comparing theoretical and simulation results, we try to establish the relationship between two parameters numerically. This can increase greatly the versatility of the lattice-based Monte Carlo simulation methods to be straightforwardly applied to more realistic diffusion-reaction systems.

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장소: 제주ICC

발표코드: I -PHYS.P-112

발표분야: 물리화학

발표종류: 포스터, 발표일시: 목 10:30~12:30

## **Anisotropic diffusion effects on the diffusion-reaction systems**

홍우식, 김효준

동아대 화학과

Monte Carlo simulation method is one of the simplest numerical experiments to obtain the probability distribution statistically. We find that the value of a diffusion constant can be controlled by changing the probability ratio of the stay to the movement in the lattice-based Monte Carlo simulations. In two or three dimensions, we can simulate the anisotropic diffusion-reaction systems by using the different probability ratio for each coordinate. The accuracy of Monte Carlo methods can be confirmed by reproducing the theoretical predictions in isotropic diffusion-reaction systems. Simulation results are easily obtained and compared in anisotropic systems where theoretical predictions are absent.

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장소: 제주ICC

발표코드: I-PHYS.P-113

발표분야: 물리화학

발표종류: 포스터, 발표일시: 목 10:30~12:30

## Nano-interface Junction Technology Using Hard and Soft Phase Magnetic Materials

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. Homogeneously dispersed nanoparticles of hard phase (NdFeB, SmCo5) were prepared by thermal decomposition method while soft phase magnetic material (Fe<sub>3</sub>O<sub>4</sub>) 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.

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장소: 제주ICC

발표코드: I-PHYS.P-114

발표분야: 물리화학

발표종류: 포스터, 발표일시: 목 10:30~12:30

## Synthesis of Tungsten Trioxide Monohydrate Nanoplate by Hydrothermal

Song guang, 강영수

서강대 화학과

Tungsten trioxide (hydrates) nanoplates were synthesized under highly acidic condition by a simple hydrothermal method. Lactic acid has been used as a fundamental agent in the formation of plate shape. Different experiment conditions, such as concentration, pH of the precursor, reaction time and reaction temperature, have been checked to find the growth process and limit of the nanoplates. The products have been characterized by X-Ray Diffraction and Scanning Electron Microscope. The results indicated that the crystal phase is orthorhombic and the particle size is about 400x400x100 nm. Keywords: Tungsten trioxide, Lactic acid, nanoplate, hydrothermal

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장소: 제주ICC

발표코드: I-PHYS.P-115

발표분야: 물리화학

발표종류: 포스터, 발표일시: 목 10:30~12:30

## Host-Guest complexation dependence of dissociation constant of 2-nitro-1-naphthol with $\beta$ -Cyclodextrin

정하영, \*김명화

이화여대 화학과 \*이화여대 화학 나노과학과

We study the shift of the dissociation constant of a 2-nitro-1-naphthol by the non-covalent interaction with  $\beta$ -Cyclodextrin ( $\beta$ -CD) using absorption and fluorescence spectroscopy. The temperature dependence of the dissociation constant of 2-nitro-1-naphthol was first spectrophotometrically determined between 10oC and 50oC in cacodylate buffer solutions. The binding constant of 2-nitro-1-naphthol with  $\beta$ -CD for 1:1 complex formation was then obtained from the enhancement of fluorescence with the increase of the concentration of  $\beta$ -CD up to 10mM. The ground-state pKa values of a 2-nitro-1-naphthol have been also estimated in the presence of varying concentration of  $\beta$ -CD. We found that the measured pKa in the presence of  $\beta$ -CD is much lower than pKa value measured in the absence of  $\beta$ -CD. This pKa shift of 2-nitro-1-naphthol arises from the differential affinity of the host molecule to encapsulate the deprotonated and neutral form of a 2-nitro-1-naphthol.



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발표분야: 물리화학

발표종류: 포스터, 발표일시: 목 10:30~12:30

## Variation of Surface-Enhanced Raman Spectra of Catecholamine Neurotransmitters Adsorbed on Silver Surface

이지훈, 이승장, 이영, 최현경, 정병서, 조한국

인천대 화학과

Raman spectra of catecholamine neurotransmitters, dopamine and epinephrine, have been studied by Surface-Enhanced Raman Spectroscopy (SERS) with the aim of possible application of the SERS technique for trace analysis of neurotransmitters. The SERS spectra of dopamine and epinephrine have been obtained using various silver colloids and SERS samples prepared by several different methods. While dopamine and epinephrine all show similar spectra with the Raman bands reflecting catechol ring vibrations and carbon-oxygen stretches, drastic changes in the SERS spectra have been observed with several new emerging bands depending on the neurotransmitter concentration and the condition of SERS substrates. We have also investigated the effects of types and concentrations of aggregating agents on the variation of spectra as well as the enhancement of Raman sensitivity. These spectral variations are interpreted in terms of interactions between neurotransmitters and metal surface leading to aggregation and/or specific molecular orientations on metal surface.

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발표코드: I-PHYS.P-117

발표분야: 물리화학

발표종류: 포스터, 발표일시: 목 10:30~12:30

## **Vibrational Analyses and Molecular Geometries of Natural Dyes on Silver Surface Based on the Enhanced Raman Spectra**

허진영, 전해선, 조창호, 정병서, 조한국

인천대 화학과

The huge enhancement of Raman scattering and suppression of fluorescence on metal surface provide a powerful means for the analysis of trace elements, such as detection of natural dyes in archeological textiles, painting, and other art works. In principle the vibrational mode perpendicular to the surface shows a large magnitude of enhancement and frequency shift. In this study the SERS spectra of juglone and lawsone, two well known natural dyes with similar molecular structures, are investigated. The optimum conditions for analysis of these natural dyes have been searched. While the strong bands at  $\sim 1670\text{ cm}^{-1}$  in their infrared and FT-Raman spectra are missing in the SERS spectra, new strong bands appear on the red side. The observed SERS bands are interpreted on the basis of the previous spectroscopic studies and DFT computation results for various molecular orientations on Ag surface. The best agreement was obtained with the dye molecule coordinated to an adatom, parallel to the earlier results for similar molecular systems.

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발표코드: I-PHYS.P-118

발표분야: 물리화학

발표종류: 포스터, 발표일시: 목 10:30~12:30

## **Molecular Dynamics Simulations of Self-assembled Helical Tubules: chirality inversion and diameter change**

이동선, \*이명수, 석차욱

서울대 화학부 \*서울대 화학과

Molecular dynamics simulations were performed for helical tubular shaped supramolecules obtained by self-assembly of small block molecules based on an m-linked aromatic segment in aqueous solution. Chirality and diameter of the tubule change with temperature as observed from TEM images and CD spectra, and computational analysis was focused on explaining the two different assembly structures. In order to understand the changes in atomic details, molecular dynamics simulations in explicit water environment using GROMACS were performed with different initial structures and parameter sets. From these simulations, we suggest molecular models for the tubular structures of large and small diameters that show chirality inversion. Detailed analysis of the structures lead to explanations of the changes in terms of polar interactions among the pyridine ring, the terminal aldehyde group, and the polar coils. Experimentally observed hydrogen bonding properties of the assemblies can also be explained with the models.

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장소: 제주ICC

발표코드: I-PHYS.P-119

발표분야: 물리화학

발표종류: 포스터, 발표일시: 목 10:30~12:30

## **Docking ligands onto flexible receptor proteins using conformational space annealing**

신용희, 허림, 석차욱

서울대 화학부

Protein-ligand docking techniques are one of the essential tools for structure-based drug design. Although conformational changes frequently occur in the binding process, many docking programs ignore receptor flexibility. We previously developed a docking program called LigDockCSA, which searches the conformational space using conformational space annealing with the LigDock scoring function that combines AutoDock3 and PLP scoring functions. However, LigDockCSA also treated the receptor proteins rigid. Here, we present an extension of LigDockCSA that accounts for side chain flexibility in the ligand-binding site. To test the performance of the new docking method, protein-ligand complexes that shares similar backbone structure but have different side chain conformations were cross-docked. Consideration of side chain flexibility produced promising results in this cross-docking test.

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장소: 제주ICC

발표코드: I-PHYS.P-120

발표분야: 물리화학

발표종류: 포스터, 발표일시: 목 10:30~12:30

## Computational Study of the High-Affinity Microtubule-Binding Domain of Dynein

최정현, 석차욱

서울대 화학부

Dynein is a motor protein that transports cellular cargo towards the minus end of the microtubule (MT) by consuming ATP. Cytoplasmic dynein has two heavy chains, each of which is composed of a cargo-binding tail, a ring-like head containing six AAA+ domains, and a ~15 nm stalk that has a microtubule-binding domain (MTBD) at its tip. It has been revealed that coiled-coil structure of the stalk makes a registry shift to control its affinity to MT by previous experimental studies (Kon et al. 2009, Nat Struct Mol Biol, 16(3):325-333). Recently the crystal structure of the low-affinity form of MTBD was published (Andrew P. Carter, et al. 2008, Science, 322: 1691-1695). However, high-resolution structure of the high-affinity form with shifted registry is not available yet. In this study, we generated molecular model structures for the high affinity form of MTBD by combining computational methods and previously revealed experimental data. Information on the conformational changes of MTBD was obtained by using the anisotropic network model, and candidates for all-atom model structures of MT-MTBD complex structures were generated. The conformational changes observed in the models are discussed in relation to the previous alanine mutation studies on candidate microtubule-binding helices.

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장소: 제주ICC

발표코드: I-PHYS.P-121

발표분야: 물리화학

발표종류: 포스터, 발표일시: 목 10:30~12:30

## Vertically Aligned Single-Crystalline TiO<sub>2</sub> Nanorods on Transparent Conducting Electrode for Dye Sensitized Solar Cell

강동인, 강영수

서강대 화학과

Vertically aligned single-crystalline TiO<sub>2</sub> nanorods on transparent conducting electrode was prepared from titanium butoxide, titanium tetrachloride and hydrochloric acid using solvothermal process. The length of TiO<sub>2</sub> nanorods is controlled for dye sensitized solar cell. Their diameter of TiO<sub>2</sub> nanorods was controlled for highest efficiency of photoelectrical properties and was characterized for application of dye sensitized solar cell. TiO<sub>2</sub> nanorod arrays were grown up to up to 9.5  $\mu\text{m}$  on TCO glass. The as-prepared longer nanorods may provide the larger surface area with the direct electron pathways. Keywords: Nanorods, Titania

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장소: 제주ICC

발표코드: I-PHYS.P-122

발표분야: 물리화학

발표종류: 포스터, 발표일시: 목 10:30~12:30

## Proton Transfer from the Inactive Gas-Phase Nicotine:Structure to the Bioactive Aqueous-Phase Structure

김주영, \*이성렬

경희대 일반대학원 화학과 \*경희대 응용화학과

The role of water in the structural change of nicotine from its inactive form in the gas phase to its bioactive form in aqueous solution has been investigated by two complementary theoretical approaches, geometry optimizations and molecular dynamics. Structures of the lowest-energy nicotineH<sup>+</sup>-(H<sub>2</sub>O)<sub>n</sub> complexes protonated either on the pyridine (inactive form) or pyrrolidine (active form) ring have been calculated, as well as the free-energy barriers for the proton-transfer tautomerization between the two cycles. These structures show chains of 2-4 water molecules bridging the two protonation sites. The roomtemperature free-energy barrier to tautomerization along the minimum-energy path from the pyridine to the pyrrolidine cycle drops rapidly when the number of water molecules increases from 0 to 4, but still remains rather high, indicating that the proton transfer is a rather difficult and rare event. We compare results obtained through this explicit water molecule approach to those obtained by means of continuum methods. CPMD simulations of the proton-transfer process in bulk with explicit water molecules have been conducted at room temperature. No spontaneous proton transfers have been observed during the dynamics, and biased CPMD simulations have therefore been performed in order to measure the free-energy profile of the proton transfer in the aqueous phase and to reveal the proton-transfer mechanism through water bridges. The MD bias involves pulling the proton from the pyridine ring to the surrounding bulk. Dynamics show that this triggers the tautomerization toward the pyrrolidine ring, proceeding without energy barrier. The proton transfer is extremely fast, and protonation of the pyrrolidine ring was achieved within 0.5 ps.

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발표코드: I-PHYS.P-123

발표분야: 물리화학

발표종류: 포스터, 발표일시: 목 10:30~12:30

## In- and Post-Source Decays of Peptide ions in Matrix-Assisted Laser Desorption Ionization Time-of-Flight Mass Spectrometry: Effective Temperature and Influence of Basic Residues

윤소희, \*문정희, \*\*김명수

한국표준과학연구원 미래융합기술부 \*한국생명공학연구원 단백질의학연구센터 \*\*서울대 화학부

In-source decay (ISD) and post-source decay (PSD) of peptide ions  $[Y_5X + H]^+$ ,  $[XY_5 + H]^+$ ,  $[Y_2XY_3 + H]^+$ , and  $[XY_4X + H]^+$  ( $X$  = tyrosine ( $Y$ ), histidine ( $H$ ), lysine ( $K$ ), and arginine ( $R$ ) with  $H$  for the ionizing proton) generated by matrix-assisted laser desorption ionization (MALDI) were investigated with time-of-flight (TOF) mass spectrometry.  $\alpha$ -Cyano-4-hydroxycinnamic acid was used as matrix. For all ions, ISD yield was unaffected by delay time, indicating rapid termination of ISD. This was taken as evidence for rapid expansion cooling of hot 'early' plume formed in MALDI. The 'early' plume temperature estimated utilizing previous kinetic results was 800-900 K, vs. 400-500 K for 'late' plume. The results support our previous finding that the temperature of peptide ions interrogated by tandem mass spectrometry was lower than most rough estimates of MALDI temperature. Product abundance became smaller in the presence of basic residues ( $H$ ,  $K$ , and  $R$ ), in the order  $Y > H \approx K > R$ . In particular, product abundances in ISD of peptide ions with  $R$  were smaller than those with  $H$  or  $K$  by an order of magnitude, which, in turn, were smaller than that for  $[Y_6 + H]^+$  by an order of magnitude. Product abundance was affected by the most basic residue when more than one basic residue was present. Dramatic disparity in product abundance was found to arise from small difference in critical energy and entropy. Results indicate similar transition structures regardless of basic residues present, where the ionizing proton keeps interacting with a basic site.



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장소: 제주ICC

발표코드: I-PHYS.P-124

발표분야: 물리화학

발표종류: 포스터, 발표일시: 목 10:30~12:30

## Study on the Photoelectrochemical Properties of TiO<sub>2</sub> (Nanorod)/Fe<sub>2</sub>O<sub>3</sub> (Single Crystal) Electrode

차현길, 노현석, 강영수

서강대 화학과

The titania nanorods with various sizes were prepared on the surface of hematite single crystal monolayer via oblique angle deposition. The samples are characterized by X-ray diffraction, scanning electron microscopy (SEM), transmission electron microscopy. The results indicated that the as-prepared samples are titania nanorods on the surface of hematite single crystals. The effect of titania nanorod size on the hematite monolayer for photoelectrochemical properties and mechanism for charge carrier transportation pathway have been investigated on the basis of a series of I-V results. The UV-vis measurement suggests that the as-synthesized samples with different size possess different optical properties.

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발표코드: I-PHYS.P-125

발표분야: 물리화학

발표종류: 포스터, 발표일시: 목 10:30~12:30

## Morphology Control of Cuprous Oxide Crystal and Its Magnetic Properties

손종화, \*강영수

서강대 화학과 나노구조물연구실 \*서강대 화학과

Various morphology of cuprous oxide ( $\text{Cu}_2\text{O}$ ) single crystals were fabricated by precipitation method using PVP (polyvinylpyrrolidone). Hydrazine and ascorbic acid were used reducing agent for synthesizing non-surfactant used cuprous oxide. Crystal size shows around 500 nm with narrow size distribution. Samples were characterized with SEM, TEM (HR-TEM), XRD, UV, and Squid. In non-surfactant case, octahedral cuprous oxide which (111) plane is dominant and shows higher surface activities comparing with cubic one. And they also show different magnetic property.

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장소: 제주ICC

발표코드: I-PHYS.P-126

발표분야: 물리화학

발표종류: 포스터, 발표일시: 목 10:30~12:30

## Gas phase H-atom abstraction by a radical in a helical peptide and random peptide sequence

이지혜, 박혜연, 문봉진, 오한빈

서강대 화학과

기체상태 peptide 의 이차구조 차이에 따른 H-abstraction 라디칼 형성 화학 반응의 Energetics 를 TEMPO-based FRIPS 방법을 통해 밝힌 연구 결과를 발표하고자 한다. 펩타이드 이차구조가 달라지면 펩타이드 골격의 아미노기의 수소결합 양태에 따라 달라지며, H-결합에너지가 달라지게 된다. 기체상태에서 이차구조가 다르다고 알려진 헬릭스 구조 펩타이드 (AAAAAAAAAAR)와 랜덤코일 펩타이드 (RAAAAAAAAAAA)의 N-말단에 라디칼을 형성할 수 있는 자유 라디칼 개시제 2-[(2,2,6,6-tetramethylpiperidin-1-oxyl)methyl]benzoic acid 를 결합시킨 후, 충돌에너지를 주어 N-말단에 라디칼을 형성한다. 다시 이 라디칼이 붙어 있는 펩타이드에 각기 다른 충돌에너지를 주면서 펩타이드가 골격분해가 일어나는 것을 관측하고, Breakdown curve 를 각각의 펩타이드에 대해 측정하였다. 이 Breakdown curve 는 각각의 펩타이드에 따른 H-abstraction 결합에너지에 대한 값을 주었다. 자세한 실험 결과는 심포지엄에서 밝히고자 한다. 한국 연구재단의 지원(KRF-2008-314-C00166)을 받았습니다.

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## Synthesis of Li Doped Hexagonal ZnO Particles 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. Pure ZnO is n-type semiconductor and Li doped ZnO is p-type materials. We can study this type of p-n junction diode material for photocatalytic activity, degradation of toxic organic pollutants (acetaldehyde, isopropyl alcohol), oxidation of water to gaseous oxygen and photocurrent generation, all under visible light. Here we describe the synthesis and mechanism of formation of the Li-doped hexagonal ZnO nanoparticles, which is act as p-type materials. Keywords: artificial photosynthesis, p-type semiconductor, Li doped ZnO

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## Polymethacrylate-based monolithic capillary columns for the separation of peptides

소혜림, 오한빈

서강대 화학과

Polymethacrylate-based monolithic capillary column 을 자체 제작하여 펩타이드들을 분리 분석하였다. Polymethacrylate-based monolithic capillary column 은 thermal-polymerization 방법에 의해 제작되었으며, monomer 로써 butyl, hexyl, lauryl, stearyl methacrylate 등을 사용하였다. Cross-linker 로 Ethylene dimethacrylate (EDMA)을 이용하였고, 반응의 initiator 로 2-2'-azobisisobutyronitrile (AIBN)를 사용하였다. Polymerization mixture 에서 어떤 monomer 를 선택하는지에 따라 탄소 사슬의 길이가 달라져 polymer 의 소수성을 조절할 수 있으며, 따라서 peptide 의 분리에 영향을 미치게 됨을 확인할 수 있었다. 본 연구에 의해 자체 제작된 monolithic column 은 향후 다양한 프로티오믹스 LC-MS 연구에 활용될 계획이다. 이 연구는 한국 연구 재단(KRF-2008-314-C00166)의 지원을 받았습니다.

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## Morphology Control Metal Doped Fe<sub>2</sub>O<sub>3</sub> Nanocrystal

노현석, 차현길, 강영수

서강대 화학과

We have developed a hydrothermal process to synthesize crystalline metal doped Fe<sub>2</sub>O<sub>3</sub> crystals and control their morphology. Metal doped hematite crystals were prepared in an aqueous solution containing iron chloride and sodium hydroxide at 150 °C for 4 h with additional transition metal solution. M:Fe<sub>2</sub>O<sub>3</sub> crystals having cubic or pointed ellipse shapes were homogeneously nucleated and precipitated in solution. Crystal growth and preferential growth faces were controlled by the concentration of adding metal solutions. Morphological control techniques in this system will contribute to the development of solution chemistry for inorganic materials and future oxide devices. Morphology and crystal structure of the obtained product was compared with XRD, TEM, SEM, and Raman spectroscopy.

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## Fabrication of Uniformed $\alpha$ -Fe<sub>2</sub>O<sub>3</sub> Particles Exposed High Photo-reactive Facets

van thanh khue, \*차현길, \*강영수

서강대 화학과 \*서강대 화학과

Hematite ( $\alpha$ -Fe<sub>2</sub>O<sub>3</sub>,  $E_g = 2.2$  eV) particles which have the exposed high reactive facets were synthesized by a very simple route under hydrothermal condition. Hydrazine (N<sub>2</sub>H<sub>4</sub>), carboxymethyl cellulose (CMC) and potassium ferricyanide(III) (K<sub>3</sub>[Fe(CN)<sub>6</sub>]) were used as capping reagents and precursor in the reaction process. The oblique parallelepiped and octahedral forms were obtained at the concentrations of hydrazine 1.32 M and 4.95 M, respectively. The influence of different reagents and precursors such as CMC, cetyltrimethyl ammonium bromide, N<sub>2</sub>H<sub>4</sub>, ammonium acetate, N,N-dimethylformamide and K<sub>3</sub>[Fe(CN)<sub>6</sub>], ferric chloride, respectively, on the final productive morphologies was also examined systematically. The results indicated that the capping reagents play an important role in the forming the particle morphology during the reaction process. The as-synthesized products were characterized by scanning electron microscopy (SEM), transmission electron microscopy (TEM), X-ray diffraction (XRD), X-ray photoelectron spectroscopy (XPS).

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## Synthesis of Iron Modified Titanate Nano Tubes for Enhanced Photo catalytic Efficiency

**Haider Zeeshan, 강영수**

서강대 화학과

Titanate Nano Tubes have gained much attention recently because of their useful applications for harvesting solar radiations as a potential source for alternative energy applications. Simple Alkaline hydrothermal method has been applied to synthesize the Nano Tubes with High Aspect Ratio. Characterization Carried by Raman, SEM, TEM, TGA and UV-Visible Absorption Spectroscopy etc. Post Synthesis washing process play an important role in the thermal stability and physico chemical properties. Loading of Iron on Titanate Nano Tubes not only increases the Thermal Stability, rather it can Tune the Electronic properties in term of Band Gap towards Red Shift and Better Efficiency for application as Photo Catalyst. Keywords: Titanate, Nano Tubes, Fe<sub>2</sub>O<sub>3</sub>. References: J. Mater. Chem. 2010, 20, 603-610 Mater. Chem. Phys. 2011, 26, 118-127 J. Coll. Interface Sci. 2007, 316, 562-569



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## Highly Aligned ZnO Nanorod Arrays by Liquid-Solid Method

Pham Quoc Long, 강영수

서강대 화학과

In this work, highly well aligned ZnO nanorod arrays were synthesized by liquid-solid method. The ZnO nanorods were grown on ITO substrate with the support of ZnO nanoseed layers. It is shown that the smooth of ZnO nanoseed layer is the important key to obtain highly aligned ZnO nanorod arrays on ITO substrate. XRD patterns of ZnO nanorods grown on ITO substrate show the high intensity peak of (0002) facet, indicating that the rods are preferentially oriented in c-axis direction. ZnO nanorods were obtained with 2.5  $\mu\text{m}$  length and 100-200 nm diameter. TEM and SAED images show the ZnO nanrods are high crystalline. Key words: Zinc oxide nanorod arrays, photocatalyst, semiconductor

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## Synthesis of Anatase TiO<sub>2</sub> Single Crystals with Exposed Various Reactive Facets for Photocatalytic Applications

Nguyen ky cuong, 차현길, 강영수

서강대 화학과

Owing to wide-ranging industrial applications and fundamental importance, tailored synthesis of well-faceted single crystals of anatase TiO<sub>2</sub> with high percentage of reactive facets has attracted much research interest. In this work, single crystalline anatase TiO<sub>2</sub> with various reactive facets have been prepared by using hydrothermal conditions with TiCl<sub>3</sub> precursor. Fluorine species (herein HF) are introduced as a stabilizing agent to reduce surface energies of anatase TiO<sub>2</sub>, especially {001} facets, which leads to large percentage of the reactive {001} facets exposed in final titania beside other reactive {010} or {110} facets. Anatase TiO<sub>2</sub> single crystals with various reactive facets are prepared first time as results of difference in reactant concentration, and dispersing agents. The “rice-like” anatase single crystals with exposed {010} and {001} facets, were prepared in the system using TiCl<sub>3</sub> precursor and HF and dispersing agent. The carboxymethyl cellulose (CMC), used as a dispersing agent, help to control the reaction rate and suppress the agglomeration of “truncated”, “rice-like” crystals. The effects of fluorine species and precursors on the quality, the morphology and crystal structure of anatase TiO<sub>2</sub> single crystals have been investigated.

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## Molecular mechanism of the redox-sensitivity of a zinc-containing anti-sigma factor RsrA

허립, 석차옥

서울대 화학부

Sigma factors play an important role in bacterial transcription by enabling specific binding of RNA polymerase to gene promoters. These factors are often regulated by anti-sigma factors. A class of anti-sigma factors that contain zinc ion are called zinc-containing anti-sigma factor (ZAS). It has been reported that some ZAS proteins release sigma factor when treated with oxidant by releasing zinc ion and forming internal disulfide bonds. This property called redox-sensitivity provides a mechanism for coping with oxidative stress by activating the transcription of antioxidant genes. Not all ZAS proteins are redox-sensitive, but what determines the redox-sensitivity is not understood yet. In this presentation, the existence of alternative zinc ion binding-sites is proposed as a determinant of redox-sensitivity. To support this proposal, we performed a comparative modeling study of redox-sensitive and redox-insensitive ZAS proteins complexed with anti-sigma factors. Three dimensional models were built, and candidates for alternative zinc binding-sites within 20 Å from the putative binding site were found. We then carried out molecular docking simulations to check the stability of the alternative zinc binding modes. Four alternative zinc binding-sites were found to be stable for the redox-sensitive rsrA, while no stable binding-site was found for the redox-insensitive chrA. From this result, we suggest the following mechanistic model for the redox-sensitivity: zinc ion binds the multiple sites probabilistically in redox-sensitive ZAS proteins, and this makes the zinc-coordinating cystein residues more susceptible to oxidation.

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## Ag Paste with Ag Nanowires

홍준익, 김상호

공주대 화학과

Traditional screen printing is still a dominant method to print electrodes on c-Si solar cells. In order to achieve higher efficiency for c-Si solar cells, modifying the electrode material is one of the key approaches. For example, shadowing loss can be reduced by fabricating high aspect ratio electrode patterns with width of finger electrode less than 80  $\mu\text{m}$ . In this study, the rheological properties of silver paste, is improved by using Ag nanowires. The printing properties including the aspect ratio of printed electrode can be improved with higher Thixotropic index (T.I.) values.

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## Modification of silver nanowires

박미선, 김상호

공주대 화학과

From liquid crystal display (LCD) and touch panels, solar cells and more, indium tin oxide (ITO) is extensively used as the material for transparent electrodes. Although new transparent electrode materials are reaching the level of practical use now, we will replace ITO thanks to characteristics including improved flexible, lower cost and higher transmittance. However, ITO film is necessary to development of alternative materials due to the scarcity of indium and durable of ITO. When applied as a coating to glass or film include silver nanowires is expected conductive, highly transparent surfaces which reflect infrared rays while allowing visible light and ultraviolet rays to pass. Au or Ag was coated on the silver nanowires because the problems of silver oxidation in air.

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## **Flexible and Highly Conductive Transparent Electrode using Silver Nanowires**

서동민, 배창완, 김상호

공주대 화학과

As displays become larger and solar cells become cheaper, there is an increasing need for low-cost transparent electrodes. Various types of transparent and conductive oxides (TCO) have been widely used in optoelectronics, such as indium tin oxide (ITO). However, there has been an increasing need to replace ITO based TCO due to the exhaustion of Indium material and flexibility problem of ITO films. Here, we report a novel transparent electrode based on Ag nanowires. Ag nanowires are synthesized with diameter less than 100 nm and length bigger than 50  $\mu\text{m}$ . The Ag nanowires are coated onto PET films and the resulting TCO shows 50 ohm/ $\square$  resistance and > 80% optical transmittance.

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## **Rheological behaviors of Ag nanowire dispersions and reversible arrangement and disordering of Ag nanowires in a shear field**

**ZHOU HU**, 서동민, 배창완, PIAO LONGHAI, 김상호

공주대 화학과

Ag nanowires (NWs) were synthesized by a modified polyol reduction method. Stable Ag NW dispersions were obtained by adding Poly(vinyl pyrrolidone) (PVP) in batches to ethylene glycol suspensions of Ag NWs and the rheological behaviors were studied. Unlike CNT dispersions, the Ag NW dispersions did not form a physical gel even in the concentrated regime, which was ascribed to the stiffness of Ag NWs. Furthermore, their structural evolution was studied after various perturbations were introduced. It is found that the shear moduli markedly decreased after cessation of the intensive shear while their shear moduli and viscosity were able to recover to the prior state under small shear. The investigation of optical microscopy showed that the decrease and recovery of the shear moduli and viscosity was dependant on the NWs' alignment and disordering. This interesting rheological behavior was explained through the rheology of 1D particles. The stable alignment and reversible return to isotropy is unique to Ag NWs, attributable to the Brownian motion of nanometer-sized 1D particles

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## Synthesis of Water-Soluble Gadolinium Iodate Nanoparticles for MRI contrast agent

이은정, Xu Wenlong, Kattel Krishna, 박자영, 김한결, 허우철, \*Badrul Alam Bony, 이강호

경북대 화학과 \*경북대 Chemistry

Paramagnetic contrast agents are routinely used in magnetic resonance imaging, because relatively small quantities can safely be introduced, resulting in a significant spin relaxation. So, we synthesized water-soluble Gadolinium Iodate ( $\text{Gd}(\text{IO}_3)_3$ ) by using two types of ligands. Their advantages in MRI applications include high solubility in water. They have been synthesized through several steps by refluxing each of them in water and then we characterized them through HR-TEM, XRD, FT-IR, TGA, and MRI instrument.



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## Longitudinal Water Proton Relaxivities of $\text{Gd}(\text{OH})_3$ Nanorod, $\text{Gd}(\text{OH})_3$ Nanoparticle, and $\text{Gd}_2\text{O}_3$ Nanoparticle: Dependence on Particle Diameter, Composition, and Morphology

박자영, Kattel Krishna, Xu Wenlong, 김한결, 이은정, \*Badrul Alam Bony, 허우철, 이강  
호

경북대 화학과 \*경북대 Chemistry

Gd(III) ion based nanomaterials such as  $\text{Gd}(\text{OH})_3$  nanorod,  $\text{Gd}(\text{OH})_3$  nanoparticle, and  $\text{Gd}_2\text{O}_3$  nanoparticle which are important for application to highly sensitive  $T_1$  MRI contrast agents, are synthesized and their water proton relaxivities are investigated. Low transverse water proton relaxivities ( $r_2$ ) ranging from 3.4 to 16.2  $\text{s}^{-1}\text{mM}^{-1}$  are observed because all samples are paramagnetic down to  $T = 3$  K. Longitudinal water proton relaxivities ( $r_1$ ) ranging from 0.8 to 5.7  $\text{s}^{-1}\text{mM}^{-1}$  are observed, depending on particle diameter such that an optimal particle diameter ( $\approx 1.7$  nm) exists for a maximal  $r_1$  ( $\approx 15.2$   $\text{s}^{-1}\text{mM}^{-1}$ ), but do not much depend on either composition or morphology. Surface Gd(III) ions mainly contribute to the longitudinal water proton relaxation.

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## **A study of Fluorescence and water proton relaxivity properties of FITC coated gadolinium oxide nanoparticles**

**Xu Wenlong, Kattel Krishna, 박자영, 김한결, 이은정, 허우철, \*Badrul Alam Bony, 이강호**

경북대 화학과 \*경북대 Chemistry

We report a facile synthesis of PEI surface-modified Gadolinium oxide nanoparticles in buffer and later coated with Fluorescein isothiocyanate isomer (FITC) and these were found monodisperse in diameter and highly water-dispersible. They were characterized with XRD, FT-IR, TGA, Fluorescence spectrometer, TEM, SQUID magnetometer, relaxivity and MRI techniques. These nanoparticles can be used to enhance MRI contrast imaging as well as optical imaging. This dual imaging assessment will increase the possibility of an early detection of disease such as tumors and cancer.

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## **Dispersion stability of aluminum nanoparticles in organic solvent with polymeric dispersant**

김한결, \*박종일, 박자영, Kattel Krishna, Xu Wenlong, 이은정, Badrul Alam Bony, 허우철, 이강호

경북대 화학과 \*포항산업과학연구원 원천소재 연구센터

In this study, the effects of both the dispersants and their concentration on the dispersion stability of aluminum nanoparticles in isobornyl acrylate and terpineol were investigated by using a visual inspection and a backscattering profile measurement. The backscattering profiles measured by “Turbiscan” showed the variation of particle size (coalescence and sedimentation). The visual inspection also confirmed that the aluminum suspensions with dispersant were stable. The observed suspension stability of aluminum nanoparticles was attributed to the steric effect for the dispersant.

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## Salt effects on the physical properties of magnetite nanoparticles synthesized at different NaCl concentrations

허우철, 박자영, Kattel Krishna, Xu Wenlong, 김한결, 이은정, \*Badrul Alam Bony, 이강호

경북대 화학과 \*경북대 Chemistry

Magnetite nanoparticles were synthesized at a wide range of NaCl solutions ( $c=0.01-3.0\text{M}$ ) and their physical properties were investigated. The particle diameter ( $d$ ) was reduced from 7.7 to 6.8 nm and the colloidal stability dropped with increasing  $c$ . The saturation magnetization ( $M_s$ ) reduction and the lattice contraction ( $\Delta a$ ) from  $-0.015$  to  $-0.038 \text{ \AA}$  with increasing  $c$  were observed due to the decrease of the  $d$ . From the  $\Delta a$ , the surface tension ( $\gamma$ ) enhancement from 0.192 to 0.614 N/m with increasing  $c$  was estimated. A simple formula which satisfactorily explains the observed salt effect on the  $d$ , is proposed from a homogeneous nucleation model.

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## Synthesis and Characterization of Dysprosium Oxide Nanoparticles for Magnetic Resonance Imaging (MRI) Contrast Agent

**Kattel Krishna**, 박자영, Badrul Alam Bony, 김한결, 이은정, 허우철, 이강호

경북대 화학과

We present a simple one step synthesis of D-glucuronic acid coated dysprosium oxide nanoparticles and characterized them with XRD, TEM, FT-IR, TGA, SQUID magnetometer and MRI instrument. We observed the average particle diameter from 2 to 4 nm. In vitro test 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 agent.

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발표종류: 포스터, 발표일시: 목 10:30~12:30

## A Facile One-Pot Synthesis of Water Soluble MnO Nanocolloid for Molecular T<sub>1</sub> MR Imaging

**Badrul Alam Bony**, \*박자영, \*Kattel Krishna, \*Xu Wenlong, \*김한결, \*이은정, \*허우철

경북대 Chemistry \*경북대 화학과

A facile one-pot synthesis of D-glucuronic acid coated MnO nanocolloid is reported. The MnO nanoparticle was coated with a biocompatible and hydrophilic D-glucuronic acid and its particle diameter was nearly monodisperse and ranged from 2 to 3 nm. The MnO nanoparticle was nearly paramagnetic below 3K temperature. The MnO nanocolloid showed a high longitudinal water proton relaxivity as well as high surface to volume ratio of the MnO nanoparticle. High  $r_1$  relaxivity of  $7.02 \text{ s}^{-1} \text{ mM}^{-1}$  was observed for MnO and this value is higher than those of the clinically used metal ion chelated MRI contrast agents. The three key parameters which control the  $r_1$  and  $r_2$  relaxivities of nanocolloids (i.e., the S value of a metal ion, the spin structure, and the surface to volume ratio of a nanoparticle) successfully accounted for the observed  $r_1$  and  $r_2$  relaxivities of the MnO nanocolloid.

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## Charge transfer enhancement in the SERS spectra of 4-aminobenzenethiol

최한규, 김지환

고려대 화학과

We investigated spatially and temporally resolved surface enhanced Raman scattering (SERS) spectra of 4-aminobenzenethiol (ABT) on Ag thin film (thickness of 10 nm). When excited with 632.8 nm laser radiation, the intensities of the  $b_2$  mode (9b, 3, and 19b) are found to increase in time, following a uni-molecular kinetics. In addition, we observe that the  $b_2$ -intensities can be locally “activated”. In both time-resolved and spatially resolved SERS measurements, the change appears to be irreversible. Additional measurements of TOF-SIMS, AFM, and optical transmission on the activated region strongly support the chemical reaction of the 4-ABT. Our observation, however, is still insufficient to unambiguously prove or disprove the recent claim by Tian and co-workers ( J. AM. CHEM. SOC. 2010, 132, 9244–9246) that the  $b_2$ -intensities originate from the SERS of the photo-product of 4-ABT. Further investigation is currently under way.

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발표종류: 포스터, 발표일시: 목 10:30~12:30

## Plasmonic Coupling between Au Film and Nanoparticles

김진욱, 권혁상, 김지환

고려대 화학과

Au nanoparticle (diameter of 100 nm) was fixed on Au thin film (thickness of 10 nm) by dispersing nanoparticles on a film. We observed ensemble averaged extinction spectra and single particle dark-field spectra in order to study the coupled plasmon resonance of nanoparticle/thin film (NPTF) junction. Distance between the Au nanoparticle and thin film is varied by spacer of different thickness (aminobenzenethiol, alkanethiols, Si thin layer). Changing distance leads to drastic change in coupled resonance wavelength. FDTD simulation reproduces the observed change numerically. Our experimental observation and electrodynamic simulation show the possibility that NPTF junction can serve as a superior plasmonic ruler than the generic ones that are made of NP dimers.



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발표종류: 포스터, 발표일시: 목 10:30~12:30

## Proton-bound Cytosine, Guanine Homo and Hetero DNA Base pairs in the gas-phase: Detailed Structure Exploration using DFT Calculations and Infrared Photodissociation Spectroscopy (IRPD)

성연미, \*한상윤, 오한빈

서강대 화학과 \*한국표준과학연구원 나노바이오융합연구단

In this study, we investigated the gas-phase structures of proton-bound DNA base pairs, particularly, cytosine and guanine, using infrared photodissociation spectroscopy (IRPDS) and B3LYP density functional theory (DFT) calculations with the basis sets of 6-31+G (d,p). In theoretical calculations, we've considered all possible DNA base combination structures, particularly taking each DNA base's diverse protonation sites and tautomeric form into account. For CC...H<sup>+</sup> and GC...H<sup>+</sup>, eighteen and twenty one base pairs combination structures were applied to the DFT calculations. The most stable structures for CC...H<sup>+</sup> was found to have three intermolecular hydrogen bonding and for the most stable GC...H<sup>+</sup> there are two hydrogen bonds. In the IRPD spectra of CC...H<sup>+</sup> and GC...H<sup>+</sup>, two absorption peaks were found; 2,903 and 3,455 cm<sup>-1</sup> in CC...H<sup>+</sup> and 3,210 and 3,520 cm<sup>-1</sup> in GC...H<sup>+</sup>. The theoretical vibration spectra showed good similarity to the previously obtained experimental spectra. This work is financially supported by the National Research Foundation of Korea (NRF-2009-0075245).

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## Ag Nano Ink for c-Silicon Solar cell

유은결, 김상호

공주대 화학과

Electrode is one of the key element in c-silicon solar cells. In order to form front silver electrode, silver paste is screen printed onto solar cell wafer and heat-treated at high temperature ( $> 800^{\circ}\text{C}$ ). Since this conventional metalization process makes contact to the wafers during the process, it may damage the wafer and sometimes break them. Especially, solar wafers being thinner and thinner to reduce wafer cost, this contact printing process will become more problematic. Therefore, an alternative process using inkjet printing process has been intensively studied. In this study, silver nano ink was prepared for the inkjet printing of solar cells. Unlike the typical inkjet ink, this study includes nano-size glass frit to etch the  $\text{SiNx}$  anti-reflection layer. Using this ink, we can fabricate solar cells without additional  $\text{SiNx}$  etching processes

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발표종류: 포스터, 발표일시: 목 10:30~12:30

## **Fabrication and Characterization of Single-Crystalline Au Nanowire Electrodes**

강미정, 강태준, 곽주현, 김봉수

KAIST 화학과

Single nanowire electrode (NWE) was fabricated by using a single-crystalline Au nanowire (NW). In order to fabricate a single Au NWE, we synthesized Au NWs by vapor transport method without any catalyst and manipulated a single NW through optical microscope combined with a custom-built nanomanipulator. The successful fabrication of a NWE was confirmed by cyclic voltammetry measurements of oxidation and reduction of a Au NW. We also obtained a sigmoidal and steady-state cyclic voltammogram of ferricyanide. Furthermore, the surface of a Au NWE can be modified by dye-labeled DNA, suggesting potential applications of single Au NWE to drug delivery into biological substances.

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## **The ab initio quantum mechanical investigation for $(\text{H}_2\text{O}_3)_n$ ( $n = 1 - 5$ ) clusters**

서현일, 김승준

한남대 화학과

We have studied molecular structures, energetics and vibrational frequencies of trioxidane,  $(\text{H}_2\text{O}_3)_n$  ( $n = 1 - 5$ ), using density functional theory(DFT) with large basis sets. The highest level of theory employed in this study is B3LYP/aug-cc-pVTZ. The geometrical parameters of trioxane clusters are predicted to have two isomers, one of which is linear while other is ring isomer. We found the new global minimum, cis ring structure, at  $n \geq 4$  which was not predicted previously. Harmonic vibrational frequencies and IR intensities are also determined at the same level of theory and confirm that all the optimized geometries are true minima.

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## Synthesis and Characterization of Naphthalic Amide Derivatives having Metal Ion-Sensing Ability

Minh Phung Doan, \*정우철, \*\*전기석, \*\*\*최창식, \*이기환

Longan department of natural resource and environment \*공주대 화학과 \*\*한국화학연구원 나노바이오융합연구센터 \*\*\*극동대 한약자원학과

To learn emission behaviors of Naphthalic Amide Derivatives, we have been simply and systematically synthesized the aromatic amide conjugated systems showing the emission property by the connection of amide bond through one-pot condensation reaction. Various functional parts like electron withdrawing group ( $X = F, Cl, NO_2$ ) and electron donating group ( $X = CH_3, OCH_3, N(CH_3)_2$ ) were introduced into the structural architecture to develop the smart and highly emissive photo-materials. The surface morphologies of the synthesized compounds were characterized by using SEM images. The effect of various metal cations upon the absorbed and fluorescent intensity have been studied in detail in ethanol solution. The fluorescent intensity of N-p-nitrophenyl-2-naphthyl amide increases in the presence of metal ions ( $Na^+$ ,  $Ca^{2+}$ ,  $Mg^{2+}$ ,  $Cr^{3+}$ ,  $Fe^{3+}$ ) due to the complex formation between the added metal ion and the unshared electron pair from the nitrogen atoms, suggesting that it could be used as ON-OFF analytical devices for signalling the presence of protons.

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## Detection of Single Nucleotide Polymorphism by Au Nanowire-on-Film SERS Sensor Coupled with S1 Nuclease Treatment

강태준, 김봉수

KAIST 화학과

Single nucleotide polymorphisms (SNPs) can serve as important biomarkers for genetic diseases, for which accurate detection of SNPs is essential for early diagnosis. We have developed a novel SNPs sensor by combining Au nanowire (NW)-on-film surface-enhanced Raman scattering (SERS) platform with S1 nuclease reaction. The combined sensor system provides reproducible SERS signals only in the presence of perfectly matched target DNAs to probe DNAs as a result of single stranded DNA (ssDNA)-specific degradation by S1 nuclease. Furthermore, point mutations in DNAs causing Wilson disease (WD) and Avellino corneal dystrophy (ACD) were successfully identified by this sensor, indicating its practical ability to diagnose genetic diseases.

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## An NMR study of deuterium diffusion in $\text{Zr}_2\text{NiD}_{4.8}$

김철, \*Son-Jong Hwang

한남대 화학과 \*Division of Chemistry and Chemical Engineering, California Institute of Technology

$\text{Zr}_2\text{Ni}$  is an intermetallic compound with the  $\text{Al}_2\text{Cu}$  structure, space group  $I4/mcm$ .  $\text{Zr}_2\text{Ni}$  absorbs deuterium to the composition  $\text{Zr}_2\text{NiD}_{\sim 5}$  and slightly deforms and in  $\text{Zr}_2\text{NiD}_{4.8}$  it was suggested to have an orthorhombic supercell structure as a result of deuterium ordering.  $\text{Zr}_2\text{Ni}$  contains four types of tetrahedral interstices that are candidates for deuterium occupation. Two of them (16(l) and 4(b) sites of Wyckoff positions) are coordinated by four Zr atoms and the 32(m) site is coordinated by three Zr and one Ni atoms, and 16(k) is coordinated by two Zr and two Ni atoms. The occupation numbers of deuterium atoms and the diffusion rates among the four sites was investigated by measuring the deuterium NMR spectra in the range of temperature of 193 K to 310 K. deuterium was found to occupy the 13%, 30%, 35%, 48% of 16k, 32m, 16l, and 4b sites, respectively, at low temperature but deuterium As the temperature increases and the deuterium atoms diffuse into other interstitial sites, the deuterium SSNMR peaks merged to each other and finally coalesced into one peak over 245 K. from the computer simulation for the deuterium diffusion among the four sites, The deuterium hopping rate was measured to be about  $5 \times 10^3$  Hz at 245 K.

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## Low-temperature reduction of NO on rutile $\text{TiO}_2(110)\text{-}1\times 1$

김보성, 김유권, \*Zhenjun Lee, \*Bruce D. Kay, \*Zdenek Dohnálek

아주대 자연과학부 \*Pacific Northwest National Laboratory, USA

In this study, temperature-programmed desorption (TPD) is employed to explore catalytic reduction of NO over rutile  $\text{TiO}_2(110)\text{-}1\times 1$ . It is found that NO readily reacts on  $\text{TiO}_2(110)$  to induce a desorption of molecular  $\text{N}_2\text{O}$  leaving oxygen adatom behind even at the substrate temperature as low as 70 K. At the substrate temperature of 70 - 150 K, the reaction rate is measured as a function of time at the beam flux of  $\sim 1\times 10^{14}$  NO/cm<sup>2</sup>sec and is found to show a sharp increase as soon as the beam is open, which decreases exponentially as the oxygen adatom builds up on the surface and the surface NO concentration reaches a saturation. The reaction is investigated further to understand its relation to the surface structure of  $\text{TiO}_2(110)$ . The subsequent TPD shows additional  $\text{N}_2\text{O}$  desorption channels up to 400 K. The observed results are explained from the role played by  $\text{Ti}^{4+}$  sites and the charge induced by oxygen vacancies and subsurface  $\text{Ti}^{3+}$  interstitials.



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발표종류: 포스터, 발표일시: 목 10:30~12:30

## Highly Conductive Lead Chalcogenide Quantum Dot Solids Somyung Jeong and Sohee Jeong

정소명

충북대 화학과

Electrical conductivity in quantum dot solids is crucial for application in devices. In addition to the wellknownligand exchange strategies for enhanced conductivity, the current study examined the optical, structural,and electrical properties of ethanedithiol-treated layer-by-layer (LbL) assembled quantum dot solid (QDS)films following low-temperature annealing (room temperature to 170 °C). As the annealing temperature increased, it was induced that the average separation between nanocrystal quantum dots is decreased, andaccordingly, the overall conductivity of the QDS increased exponentially. From a simplified percolation model,the activation energy of temperature-dependent quantum dot attachment was estimated to be around 0.26-0.27 eV both for PbS and PbSe quantum dot solids. Furthermore, the results of this study indicated that deviceapplications requiring higher conductivity, attainable through high-temperature annealing, may also requirerepassivation after annealing.

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## 고에너지전자빔(HEEB) 조사를 통한 플라즈마 폴리머 표면의 개질 및 바이오 응용 연구

조상진, 부진효

성균관대 화학과

The plasma polymer thin films were deposited on Si(100) substrate by PECVD (plasma enhanced chemical vapor deposition) method. Liquid cyclohexene was used as single organic precursor. It was heated up to 60 °C and bubbled up by hydrogen gas, which flow rate was 50 sccm (standard cubic centimeters per min.). Deposition temperature was room temperature. Plasma was ignited by radio frequency (RF; 13.56 MHz) of 10 W. As-deposited plasma-polymer thin films were treated by e-beam of 300 keV with various adsorption radiation doses. The plasma polymer films, which were treated by high energy e-beam (HEEB), were investigated by FT-IR (Fourier Transform Infrared), XPS (X-ray Photoelectron Spectroscopy), AFM (Atomic Force Microscopy), and the water contact angles. From IR spectra, the intensity of -OH functional group is increased by increasing electron dose rate. XPS results also show that the intensity of O1s peak is increased by increasing electron dose rate. C1s peak shows that oxygen bonded at carbon site. The water contact angles are decreased by increasing electron dose rate. From the AFM analysis, we observed the formation of  $\lambda$ -DNA (Deoxyribonucleic acid) array on plasma polymer film, which was treated by HEEB with the 14 kGy of adsorption radiation dose.

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## Resonance Enhanced Multi-Photon Ionization (REMPI) and Double Resonance (UV-UV and IR-UV) Spectroscopic Investigation Isocytosine

이승준, 민아름, 김유식, 최명룡, \*Shun-ichi Ishiuchi, \*Masaaki Fujii

경상대 화학과 \*Tokyo Institute of Technology, Chemical Resources Laboratory, Japan

Isocytosine(iC), 2-aminouracil, is a non-natural nucleobase and its functional group's positions resemble those of guanine; therefore, its spectroscopic investigation is worthy of attention especially for the natural/unnatural base pairs with guanine and isoguanine. In this study, resonance enhanced multi-photon ionization (REMPI) and UV/IR-UV double resonance spectra of iC in the gas phase are presented. The collaboration work between Tokyo Institute of Technology, Japan and Gyeongsang National University, Korea using laser ablation and thermal evaporation, respectively, for producing jet-cooled iC is presented and discussed. The excitation REMPI spectrum of iC monomers is recorded in the spectral range of 35000 to 36400cm<sup>-1</sup>, showing very congested  $\pi$ - $\pi^*$  vibronic bands. UV-UV hole burning spectroscopy is further conducted to investigate the conformational landscapes of iC monomers. Moreover, the presence of free OH band from IR-UV double resonance spectroscopy in combination with quantum chemical calculations convinces that the iC monomer in free-jet expansion experiment is an enol tautomer.

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발표종류: 포스터, 발표일시: 목 10:30~12:30

## REMPI and UV-UV double resonance spectroscopy of 2-aminophenol

김민호, \*손운용, 박영동, 강혁

아주대 화학과 \*아주대 에너지시스템학부

The electronic spectrum of 2-aminophenol (2AP) in the gas phase has been investigated by 1-color resonance-enhanced multiphoton ionization (REMPI) and UV-UV double resonance spectroscopy and *ab initio* calculation at the second-order approximate coupled cluster (CC2) level. Two conformational isomers of 2AP are possible, *cis* and *trans* according to the orientation of OH group relative to NH<sub>2</sub> group. Our calculation indicates that the *trans* isomer is more stable than the *cis* isomer in the ground state, because the intramolecular hydrogen bonding structure in the latter involves rotation of NH<sub>2</sub> group with a high barrier. The REMPI spectrum shows the 0-0 band of 2AP at 33,450 cm<sup>-1</sup> and strong 125 cm<sup>-1</sup> progression. The 125 cm<sup>-1</sup> progression is assigned to the progression of 10a vibration (butterfly mode) based on the frequency calculation in the S<sub>1</sub> state at the CC2 level. Calculation of Franck-Condon overlap integral successfully reproduced the experimental spectrum. According to the calculation, the excitation energy of the *cis* conformer (37,986 cm<sup>-1</sup>) is much higher than that of the *trans* conformer (31,615 cm<sup>-1</sup>) in  $\pi\pi^*$  transition. UV-UV double resonance spectrum also shows that our spectrum has only *trans* conformer.

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## Solvent Assisted Conformational Isomerization of substituted phenols and anilines

손운용, \*김민호, \*강혁, \*박영동

아주대 에너지시스템학부 \*아주대 화학과

It was demonstrated that solvent-assisted conformational isomerization (SACI), which drives the population of the less stable cis isomer into the more stable trans isomer by various solvents, occurred in our previous experiments on 3-aminophenol. In order to confirm these evidences, m-anisidine (3-methoxyaniline) was investigated as an effort to tune the activation energy by replacing the hydrogen of the hydroxyl group with a heavier methyl group. Contrary to our expectation, the activation energy of anisidine is almost the same as that of 3-aminophenol, thus it showed same results with 3-aminophenol. These results signify that mass doesn't influence the activation energy significantly. 3-cyanophenol was also investigated to increase the activation energy by replacing the amino group with a cyano group. Because of an electron withdrawing effect of the cyano group, the  $\pi$  interaction between oxygen and aromatic ring becomes stronger than in 3-aminophenol. It was confirmed by our experiments and computations, and it showed that the results were different from those of 3-aminophenol.

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## Structures and Magnetic Properties of Cobalt Selenide Nanowires

고경문, 김태규

부산대 화학과

Here we exploited the Au-catalyzed vapor-liquid-solid (VLS) growth for the cobalt selenide (CoSe) nanowires through a general atmospheric pressure chemical vapor deposition (APCVD) on Au thin film coated Si (100) substrate. The growth on Au thin film coated Si (100) substrate was based on through vapor-liquid-solid (VLS) mechanism where cobalt chloride ( $\text{CoCl}_2$ ) and Selenium (Se)-graphite mixture were used 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  $\mu\text{m}$  in length. The energy dispersive x-ray spectroscopy (EDS) data indicate that the growth of CoSe nanowires shows homogeneous character. The synthesized nanowires were also investigated by x-ray diffraction (XRD) method to elucidate the detail structure of CoSe nanowires. The magnetic properties of CoSe NWs have been investigated by using superconducting quantum interference device (SQUID) magnetometer and zero-field-cooled (ZFC) and field-cooled (FC) magnetization measurements.

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발표분야: 물리화학

발표종류: 포스터, 발표일시: 목 10:30~12:30

## **Ion-pairing dynamics of $\text{Li}^+$ and anions( $\text{SCN}^-$ & $\text{SeCN}^-$ ) in dimethylformamide solution: Chemical exchange two-dimensional infrared spectroscopy**

박광희, 박성남, 조민행

고려대 화학과

Chemical exchange two-dimensional infrared (2DIR) spectroscopy is applied to investigate ion pairing dynamics occurring on picosecond timescales.  $\text{SCN}^-$  &  $\text{SeCN}^-$  ion is used as a vibrational probe. The probing anion dissolved in N,N-dimethyl formamide (DMF) has a sufficiently long vibrational lifetime and can form a contact ion pair with  $\text{Li}^+$  ion in DMF. We present experimental results on the thermal equilibrium ion pairing dynamics of  $\text{Li}^+$  and anions in N,N-dimethylformamide. The CN stretch frequency of the contact ion pair is significantly blue-shifted from that of free anions so the free anion can be spectrally distinct from the contact ion pair in DMF. We were able to directly monitor the ion pairing dynamics of  $\text{Li}^+$  and  $\text{SCN}^-$  &  $\text{SeCN}^-$  in real time by using ultrafast 2DIR spectroscopy.

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## Theoretical Study for Metal cation with benzene (M=Pb) :DFT Study

서영선, \*이철, 이기학

원광대 화학과 \*원광대 생명나노화학부

We performed to theoretical study of isomers for Pb+with Benzene complex. binding energies, corrected for zero-point energies (ZPE) and basis set superposition errors (BSSE) are calculated. The hybrid density functional theory (DFT) with Becke's three parameter hybrid method and the Lee-Yang-Parr exchange-correlation functional theory(B3LYP) were used to optimize the geometries of Pb cation with benzene isomers. The electron basis set 6-311+G\* was used throughout this work for the C, H atom and Stuttgart RLC segmented effective core potential (ECP) for Pb+metal ion. We fully optimized all geometries and using the Gaussian 03 package suite.



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## Comparison of binding mode-dependent fluorescence properties of the meso-Tetrakis(N-methylpyridinium-4-yl) porphyrin-poly[d(A-T)<sub>2</sub>] and [d(A-T)<sub>n</sub>]<sub>2</sub> oligonucleotides complexes

GONGLINDAN, 권용준, 조태섭, 김석규

영남대 화학과

Abstract Binding mode of meso-Tetrakis(N-methylpyridinium-4-yl) porphyrin (TMPyP) to poly[d(A-T)<sub>2</sub>] has been known to depend on various factors. One of the factors that affect the binding mode is the [TMPyP]/[DNA base] ratio (R ratio). At a low binding ratio, TMPyP has been known to bind across the minor groove of poly [d(A-T)<sub>2</sub>]. Upon increasing the R ratio, TMPyP start to stack moderately along the poly[d(A-T)<sub>2</sub>] stem. When the concentration of TMPyP further increases, TMPyP tends to form a TMPyP-DNA assembly, in which TMPyP stacked extensively and the DNA is believed to form a complex along porphyrin assembly. The fluorescence characteristics of the TMPyP including simple emission spectrum, fluorescence decay time, and quenching by arylamide were investigated in this work and were compared to those with the TMPyP-d[(A-T)<sub>6</sub>]<sub>2</sub> and -d[(A-T)<sub>3</sub>]<sub>2</sub>. To the former self-complementary oligonucleotide containing 12 base-pairs, TMPyP has been known to bind in the monomeric manner while to the latter oligonucleotide (6 base pairs), TMPyP purely moderately stacked. This study therefore, allows us to compare the fluorescence properties of TMPyP-poly[d(A-T)<sub>2</sub>] complex with pure monomeric and moderately stacked TMPyP along the AT base pairs. As the TMPyP-poly[d(A-T)<sub>2</sub>] complex was excited at 430 nm, it produced emission spectrum in the 600 ~ 800 nm range and was consisted of two strong bands at 654 nm and 716 nm at R ratio of 0.02. The relative intensity of these two peak namely F<sub>654nm</sub>/F<sub>716nm</sub> was 1.52. As the R ratio increased, both maxima showed the tendency to shift to long wavelength and relative ratio increased to 1.70. Both emission bands become broad with the increasing intensity around 690 nm. The emission recorded from TMPyP-oligonucleotide complex exhibited similar tendency. When TMPyP form a monomeric binding with d[(A-T)<sub>3</sub>]<sub>2</sub>, the emission bands were sharper than those stacked

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## Stacking of Zn(II)meso-tetrakis(N-methylpyridinium-4-yl)porphyrin along Z-form Poly[d(G-C)<sub>2</sub>]

GONGLINDAN, 김석규

영남대 화학과

Abstract Binding mode of water-soluble Zn(II)meso-tetrakis(N-methylpyridinium-4-yl)porphyrin (Zn(II)TMPyP) to Z- and B-form poly[d(G-C)<sub>2</sub>] and poly[d(A-T)<sub>2</sub>] at various [Zn(II)TMPyP]/[DNA] ratios, from 0.02 to 0.1, were investigated using linear and circular dichroism (LD and CD), UV and fluorescence spectroscopy. When Zn(II)TMPyP bound to B-form poly[d(G-C)<sub>2</sub>], it produced a negative CD in the Soret absorption region which is believed to be a diagnostic for intercalation binding mode. In contrast, binding of Zn(II)TMPyP to Z-form poly[d(G-C)<sub>2</sub>] and poly[d(A-T)<sub>2</sub>] produced bisignate CD spectrum, whose shape and intensity were similar in both polynucleotides, suggesting the stacking the porphyrin molecules along the polynucleotide stem in a similar manner. The spectral properties including LD, CD and UV of the complexed formed between Z-form poly[d(G-C)<sub>2</sub>] and Zn(II)TMPyP changes with time: within 48 hours, all spectral properties became similar to those of the B-form poly[d(G-C)<sub>2</sub>]-Zn(II)TMPyP complex, suggesting that Zn(II)TMPyP induces Z- to B- transition.

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발표분야: 물리화학

발표종류: 포스터, 발표일시: 목 10:30~12:30

## The effect of substituent on cyclohexanone

김지현, 가수현, 오정진

숙명여대 화학과

Many Methyl, Ethyl- substituted cyclohexanones have been studied using microwave spectroscopy and each molecule's dipole moment, spectroscopic constants, and structure parameters were determined. Because of the Methyl, Ethyl- substituted group attached at the ring, there is difference in the dipole moment value of each molecule. This difference is called induced dipole moment. In this case, cyclohexanone has a carbonyl group, and according to the result of ab initio calculation, most of dipole moment is located at the C=O bond. Thus, it is an appropriate assumption that the dipole moment of the carbonyl bond  $\mu_{C=O}=3.246$  D is the same total dipole moment  $\mu=3.246$  D of cyclohexanone. Bond moment of  $\mu_{C=O}=3.246$  D was projected to the principal axis of substituted cyclohexanones, so projection dipole moment was obtained. The difference between the experimental dipole moment and projection dipole moment is mostly from the substituted group attached at the ring in the equatorial position. In the same way, 2-methyl, 3-methyl, 4-methyl, and 4-ethyl cyclohexanone's induced dipole moments got and compared. To predict and compare the geometry parameter, ab initio calculation was performed and compared with experimental results.

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## **Synthesis of Visible Light-Sensitive ZnO Nanostructures: Optoelectronic Properties and Photocatalytic Activities**

이주란, 윤민중

충남대 화학과

Single crystalline ZnO nanowires, nanoplates and nanorods were synthesized by a sol-gel method with or without hydrothermal reaction through formation of liposome-ZnO nanocomposites, and they were characterized by measurements of XRD, SEM and TEM. The UV-Visible absorption spectra of the nanowires and nanoplates were observed to exhibit high absorption of visible light from 400 nm to 600 nm as compared to that of nanorods. In parallel with enhancement in visible light absorption, the ZnO nanostructures were observed to exhibit visible light photocatalytic activities. The optoelectronic properties of the ZnO nanostructures investigated by measuring photoluminescence (PL) spectral properties with visible light excitation at 410 nm were correlated with the structural dependence of the photocatalytic activities.

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## Surface analysis of vacuum-deposited films of Alq<sub>3</sub> derivatives

진휘원, 한진욱, \*Takashi Isoshima, \*Eisuke Ito, \*Youichi Okabayashi, \*Masahiko Hara

한양대 화학과 \*Fluto-Order Functions Research Team, RIKEN-HYU Collaboration Research Center,  
RIKEN, JAPAN

Alq<sub>3</sub> derivatives having alkyl or halogen groups on 8-hydroxyquinoline ligand were prepared and vacuum-deposited on ITO-coated glass, quartz, and silicon for surface analyses. The films were analyzed by various surface and optical analysis techniques, such as surface potential measurement by Kelvin probe, XPS, first-order electroabsorption (EA), and linear absorption and so on. Considering that Al(7-Pyq)<sub>3</sub> (Fig 1) has smaller permanent dipole moment than Alq<sub>3</sub>, the results of surface potential (Table 1) and EA measurement (Fig 2) suggest opposite sense of spontaneous polar molecular alignment and the order parameter is about three times larger than that of Alq<sub>3</sub>.

Fig 1. Al(7-Pyq)<sub>3</sub>

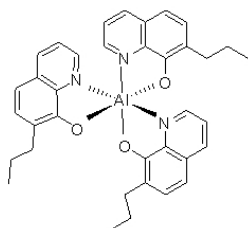
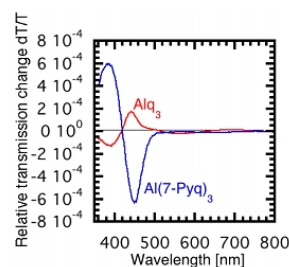


Table 1. Surface potential normalized by film thickness

| Material               | Surface potential |
|------------------------|-------------------|
| Alq <sub>3</sub>       | 43.1 V/μm         |
| Al(7-Pyq) <sub>3</sub> | -122.9 V/μm       |

Fig 2. First-order EA spectra



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## **Interaction of quercetin with metal surface studied by surface-enhanced Raman spectroscopy**

임윤성, 조한국, 정병서

인천대 화학과

Surface-enhanced Raman spectroscopy (SERS) was used for the vibrational characterization and the study of adsorption behavior of quercetin, one of the important natural dyes found in fruits and vegetables, on silver colloidal nanoparticles. The SERS spectra of quercetin were obtained using two differently prepared silver colloids, and the observed Raman bands were assigned to vibrational normal modes based on quantum chemical calculations. The SERS spectra were also obtained at different conditions of SERS substrates and at varying concentrations of aggregation agent to investigate the interaction and adsorption mechanism of quercetin on metal surfaces. The interaction of adsorbates with silver surface leading to different adsorbate conformations and/or molecular orientations were discussed based on the changes in observed SERS spectra. Also the SERS spectra of alizarin, another natural dye with related functional groups, were obtained, and comparisons were made to aid the interpretation of the quercetin spectra.

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## Computational calculations of the effects of mono-substitution on UV absorption and solubility of diketo-pyrrolo-pyrrole derivatives

김대진, 정동현, 김경현, 최승훈

(주)인실리코텍

Mono-*N*-alkylated and mono-*N*-acylated analogues of diketo-pyrrolo-pyrrole (DPP) pigments were investigated to find the relation between substituent and UV absorption using the density functional theory (DFT). In addition, molecular dynamics simulations were performed to calculate the effect of the substitution on the solubility parameters of the pigments. Time-dependant (TD) DFT method was used for the simulation of the vertical absorption spectra. Distortion of the planar geometry of DPP by the mono-*N*-alkylation does not affect the absorption spectra, but mono-*N*-acylation of DPP causes blue shift of  $\lambda_{\text{max}}$ . Solubility of mono-*N*-alkylated DPPs for ethanol, chloroform, and DMF was predicted by the molecular dynamics simulations using COMPASS forcefield. From the analysis of cohesive energy density, the solubility parameters are derived and compared with those of the solvents. The results show that the length of the substituted alkyl chain has positive correlation with the solubility.

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## Ab Initio Studies of $\beta$ -D-fluorinated glucopyranose

김진아, \*안익성, \*\*민병진

연세대 화공생명공학과 \*연세대 화공생명공학부 \*\*배재대 화학과

we have optimized conformational isomers of  $\beta$ -D-fluorinated glucopyranose using ab initio(RHF level) with 6-311++G\*\* basis set to study the conformational stability of glucopyranosides. There are a variety of inter- or intra- molecular interactions in glucopyranose according to hydroxyl groups such as gauche effect, hydrogen bonding, Exo-anomeric effect, solvation effect and so on. here we study only gauche effect from among these. Preferentially To exclude hydrogen bonding, we substitute fluore for all hydroxyl groups and pyranose ring has maintained  $4C_1$  chair conformation. Because there is no exocyclic hydroxyl groups, the conformational stability was determined by  $\omega$ -angle( $F_6-C_6-C_5-O_5$ ). To obtain the 1-D energy profile along the omega-torsion angle, we optimized the geometries at the fixed torsion angles. as a result of optimization, we could find local minimum at near the 60,180,300 degree and stabilize energy at those degree and also on the basis of newmanprojection view when C-H bond was donor, C-F bond length became longest, when C-O bond was donor, C-F bond length became shortest. Zero-point vibrational energies have been considered to predict the relative energy. Therefore the gauche effect is so for conformational isomers of  $\beta$ -D-fluorinated glucopyranose and we will discuss(frequency, spectrum,dipole moment..)



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## Real-time probing of acid-base reaction: Chemical exchange two-dimensional infrared spectroscopy

손혜원, 박성남

고려대 화학과

Acid-base reactions are of fundamental importance in chemistry, biology, and physics. Here, we have investigated acid-base reactions with hydrogen azide in methanol and dimethyl sulfoxide (DMSO) by using ultrafast two-dimensional infrared (2DIR) spectroscopy and IR pump-probe spectroscopy. The vibrational stretching frequency of  $\text{N}_3^-$ , which is peaked at  $2045\text{ cm}^{-1}$ , is significantly blue-shifted when  $\text{N}_3^-$  ion is associated with  $\text{H}^+$  ion such that  $\text{N}_3^-$  ion (basic form) and  $\text{HN}_3$  (acidic form) can be spectrally well-distinguished in the FTIR spectrum. In the present work, we measured the acid-base reaction in real-time for the first time by carrying out 2DIR spectroscopy and we also measured the population relaxation and orientational relaxation dynamics of  $\text{N}_3^-$  ion (basic form) and  $\text{HN}_3$  (acidic form) by using polarization-controlled IR pump-probe spectroscopy. By using the experimental results and the two-species exchange kinetic model, we were able to directly determine the rate constants of the acid-base reactions in methanol. The experimental results obtained with hydrogen azide in methanol and DMSO suggest that acid-base reaction in protic solvents (e.g. methanol) should occur on much faster timescales than that in aprotic solvents (e.g. DMSO). In protic solvents, the proton transfer between acidic and basic forms is assisted (catalyzed) by neighboring protic solvent molecules. On the other hand, in aprotic solvents, the proton transfer between acidic and basic forms may occur by direct transportation of the proton.

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## Dielectric Imaging of Graphene on SiO<sub>2</sub>/Si by Scattering Apertureless Near-Field Microscopy

권혁상, 김덕수, 김지환

고려대 화학과

We report the high-resolution dielectric mapping of graphene layers on SiO<sub>2</sub>/Si substrate using Apertureless Near-Field Scanning Optical Microscopy (ANSOM). The intensities and phases of scattered radiation from the tip-sample junction reflects the local dielectric functions of the sample just beneath the scanning probe and allow us to map out the dielectric constants with ~20 nm spatial resolution. The contrast dipole-image dipole model of tip-sample coupling satisfactorily reproduces the observed dielectric contrast between graphene layers and the SiO<sub>2</sub> substrate.

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## **Nafion Membrane Based Portable Membrane Introduction Time of Flight Mass Spectrometry**

김현국, 김태규

부산대 화학과

Nafion is a commercially available perfluorosulphonate cation exchange membrane commonly used as a perm-selective separator in chlor-alkali electrolyzers and as the electrolyte in solid polymer fuel cells. In this work, a Nafion sheet membrane serves as the interface between the gas stream and the vacuum in membrane introduction to the mass spectrometer (MIMS). The penetration by volatile polar compounds (VOC-methanol, ethanol, 1-propanol), volatile non-polar compounds (VOC-benzene, toluene and p-xylene), semi-volatile low polar compounds (SVOC-fluorobenzene, chlorobenzene and bromobenzene) and non-volatile polar compounds (o-chlorophenol, m-chlorophenol and p-chlorophenol) through the Nafion membrane to the mass spectrometer was studied.

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## REMPI Studies of Jet-cooled Acetaminophen-Ethanol Clusters in Gas Phase

민아름, 이승준, 김유식, 최명룡, \*김성근

경상대 화학과 \*서울대 화학부

Acetaminophen(APAP) is a widely used over-the-counter antipyretic and analgesic, a major ingredient in various cold and flu drugs, Tylenol®. There is minimal risk of side effects when it is taken as directed. However, it is well known that having it with alcohol and taking more than recommended dosages may cause a dangerous risk, such as general stomach irritation, liver failure, and in some cases, death. In a previous study, we investigated the conformational structures of jet-cooled APAP by resonance enhanced multiphoton ionization (REMPI) and UV-UV double resonance spectroscopy in the gas phase, providing the identification of two almost isoenergetic conformers, cis- and trans-APAP, in the free-jet experiments. On the basis of the results, we would like to step further on the study of APAP-ethanol clusters. In this poster, the REMPI and UV-UV hole burning spectroscopic studies of the clusters will be presented and discussed.

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## Photodissociation Dynamics of C<sub>6</sub>H<sub>5</sub>Br and C<sub>6</sub>F<sub>5</sub>Br near 234 nm by Ion-Imaging Method

폴다바브라타, 김태규

부산대 화학과

The photodissociation dynamics of bromobenzene and pentafluorobromobenzene near 234 nm have been investigated using a velocity mapping technique coupled with a state-selective [2+1] resonance-enhanced multiphoton ionization (REMPI) scheme. Tri-modal total translational energy distributions for Br(<sup>2</sup>P<sub>j</sub>, j = 1/2, 3/2) formation have been observed after the photolysis of the bromobenzene. The observed translational energy distributions have been fitted by a single Boltzmann function and two Gaussian functions. Low-velocity components with Boltzmann distributions are produced through internal conversion from the initially produced <sup>1</sup>( $\pi, \pi^*$ ) state to the vibrationally excited electronic ground state. The middle velocity components with Gaussian shapes are originated from <sup>1</sup>( $\pi, \pi^*$ ) state to <sup>3</sup>(n,  $\sigma^*$ ) repulsive state as considering predissociation of C-Br bond. The high velocity components are generated via direct dissociation by the repulsive <sup>3</sup>(n,  $\sigma^*$ ) state. The fluorination effects on the dissociation dynamics of bromobenzene high-velocity components with Gaussian shape have not been observed in the translational energy distribution of perfluorobromobenzene. The assignments of these dissociation channels also have been confirmed by the recoil anisotropy parameters of the individual components.

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## Reaction of $V^+$ ions with $(RCN)_n$ ( $R = CH_3, C_2H_5$ ) clusters: Effect of Substitution

폴다바브라타, 김태규

부산대 화학과

A laser-ablation/supersonic beam expansion method has been used to investigate the differences in clustering and reactivity of  $V^+$  ions within  $V^+(RCN)_n$  ( $R = CH_3, C_2H_5$ ) clusters. The mass spectra of the reaction of  $V^+$  ions with  $(RCN)_n$  ( $R = CH_3, C_2H_5$ ) clusters exhibit a major sequence of cluster ions with the formula  $V^+(RCN)_n$  ( $R = CH_3, C_2H_5$ ), which is attributed due to the effective ion-dipole interaction of  $V^+$  ion with RCN ( $R = CH_3, C_2H_5$ ) molecules. The other two major series of cluster ions corresponding to  $V^+(NH_2)(RCN)_n$  (primary product) and  $V^+(NH_2)_2(RCN)_n$  (secondary product) mass units in the entire spectrum are originated from the intracuster rearrangement-elimination mechanism of ion-molecule adduct via cyclic intermediate. Simultaneously, the simple ion-molecule cluster product series,  $V^+(CN)(RCN)_n$  ( $R = CH_3, C_2H_5$ ), with low intensity is attributed via electrostatically R-CN bond rupture of solvated alkanenitrile molecules followed by methyl and ethyl radical elimination. Metal or alkyl radical substitution effects are also presented.

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## REMPI and UV-UV double resonance spectroscopy of jet-cooled acetaminophen

김유식, 이승준, 민아름, 최명룡, \*김성근

경상대 화학과 \*서울대 화학부

In this work, we present the conformational investigations and photochemistry of jet-cooled acetaminophen (AAP) by resonance enhanced multiphoton ionization (REMPI) and UV-UV double resonance spectroscopy in the gas phase. AAP is a widely used antipyretic and analgesic, a major ingredient of Tylenol®. Acetaminophen consists of a benzene ring core, substituted by one hydroxyl group and the nitrogen atom of an amide group in the para pattern. In addition, DFT B3LYP calculations using the cis- and trans- form was found the presence of the AAP. And as a result of UV-UV hole burning spectroscopy have been confirmed. The 0-0 bands of cis and trans isomers of acetaminophen are found at 33517.6 and 33484.5 cm<sup>-1</sup>. Two isomers are closely laid and partially overlapped due to the small energy difference of the recorded REMPI spectrum looks very sharply congested. In the near future, IR-UV hole burning (resonant ion-dip infrared spectroscopy, RIDIRS) double resonance spectroscopy for AAP will be performed.

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## Theoretical study on the reaction of $\text{Os}^+$ with $\text{CH}_3\text{F}$ and the role of intersystem crossing

홍기룡, 김태규

부산대 화학과

$\text{Os}^+$  is known to react with  $\text{CH}_3\text{F}$  to produce  $\text{OsCHF}^+$  and  $\text{H}_2$  as primary products, but the detailed reaction mechanism and the most favorable reaction pathway have not yet been elucidated. Here we investigated the doublet, quartet, and sextet potential energy surfaces associated with the gas-phase reaction between  $\text{Os}^+$  and  $\text{CH}_3\text{F}$  for two plausible pathways, (1)  $\text{H}_2$  elimination and (2)  $\text{HF}$  elimination, by using the density functional theory (DFT) and *ab initio* methods. The molecular structures of intermediates and transition states involved in these reaction pathways are optimized at the DFT level by using the PBE0 functional. All transition states were identified by using the intrinsic reaction coordinate (IRC) method and the resulting coordinates describe how  $\text{Os}^+$  activates the C-H bond of  $\text{CH}_3\text{F}$  and yields  $\text{OsCHF}^+$  and  $\text{H}_2$  as primary products. The intersystem crossing (ISC) point is optimized by a multireference *ab initio* method, and spin-orbit effects are considered around the ISC point. On the basis of the presented results, we propose that SO induced ISC facilitates the primary  $\text{H}_2$  elimination pathway, which is less efficient in the reaction between  $\text{Fe}^+(\text{Ru}^+)$  and  $\text{CH}_3\text{F}$ .



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## Experimental and theoretical investigations of ion-molecule reactions between $\text{Ti}^+$ ion and $\text{CF}_3\text{COCH}_3$ in gas-phase

홍기룡, 김태규

부산대 화학과

The gas-phase ion-molecule reactions within  $\text{Ti}^+(\text{CF}_3\text{COCH}_3)_n$  clusters have been studied by using laser ablation-molecular beam/reflectron time-of-flight mass spectrometry. The reactions of  $\text{Ti}^+$  with  $\text{CF}_3\text{COCH}_3$  clusters were found to be dominated exclusively by an F atoms abstraction reaction, which produced  $\text{TiF}_2^+(\text{CF}_3\text{COCH}_3)_n$  clusters. These ions were attributed to the activation of a  $\text{Ti}^+$  ion onto the C-F and C=O bonds of the  $\text{CF}_3\text{COCH}_3$  molecule within five-membered association complex. In the low mass region of spectrum, both  $\text{TiF}_2^+$  and  $\text{TiO}^+$  ions are produced as competing pathways in the ion-molecule reaction between  $\text{Ti}^+$  and  $\text{CF}_3\text{COCH}_3$ . In addition, we calculated the quartet and doublet potential energy surfaces associated with the gas-phase reaction between  $\text{Ti}^+$  and  $\text{CF}_3\text{COCH}_3$  clusters for two plausible pathways. Based on the calculation results, the most favorable pathway and energetics are presented.

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## Investigation of [Cu + dCG] complexes by electrospray ionization Mass Spectrometry

이송민, 최지수, 김호태

금오공과대 응용화학과

Segments of DNA with alternating d(CG) sequences are the most favored for forming Z-DNA. At present, the data suggests that Z-DNA may play a role in the transcriptional enhancer of the DNA tumor, acting as a positive regulatory transcription signal. It is known also that Copper(II) ions play important roles to transform a general B-DNA to Z-DNA. In this study, we investigated the complex structures and binding sites of [Cu II +dCG] complex in gas-phase by electrospray ionization mass spectrometry (ESI-MS). MS/MS and MS/MS/MS fragmentation patterns of [Cu II +dCG] complex was analyzed by collision-induced dissociation (CID) method in an ion-trap LTQ mass spectrometer.

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## DNA and Porphyrin effects on Visible light Photocatalytic activities of $\text{Ag}^+$ -N-TiO<sub>2</sub> Nanochains

이형주, 윤민중

충남대 화학과

$\text{Ag}^+$ -N-TiO<sub>2</sub> nanochains had been previously fabricated and found to be the highly efficient visible light-sensitive photocatalysts and solar cells by incorporating with HPA (heteropoly phosphotungstic acid).<sup>1</sup> The HPA-incorporated  $\text{Ag}^+$ -N-TiO<sub>2</sub> nanochains demonstrated the possibility that two color-sensitive photocatalysts and solar cells mimicking Z-scheme of photoinduced electron transfer in the plant photosynthetic system. In order to develop another two-color photocatalysts and solar cells, we fabricated new composites of  $\text{Ag}^+$ -N-TiO<sub>2</sub> nanochains by employing DNA (poly d(GC) or poly d(AT))-bound porphyrins such as tetrakis (4-carboxyphenyl) porphyrin (TTCP) or tetramethyl tetraphenyl tin (Sn) - porphyrin (TTMS) instead of HPA. It was found that the photocatalytic efficiency of the nanocomposites was highly improved depending on DNA and porphyrins. The optoelectronic properties related to this finding will be discussed.

<sup>1</sup>. H. J. Lee, Ji. Lee, J. Lee, M. Yoon, J. Mater. Chem. (2011) submitted

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## **Molecular Dynamics of Carbon Nanotubes Deposited on a Silicon Surface via Collision : Temperature Dependence**

**Matin Mohammad Abdul, \*장준경**

부산대 나노융합기술학과 \*부산대 나노정보소재공학과

We investigated how temperature influences the structural and energetic dynamics of carbon nanotubes (CNTs) undergoing a high-speed impact with a Si (110) surface. By performing molecular dynamics simulations in the temperature range of 100 - 300 K, we found that a low temperature CNT ends up with a higher vibrational energy after collision than a high temperature CNT. The vibrational temperature of CNT increases by increasing the surface temperature. Overall, the structural and energy relaxation of low temperature CNTs are faster than those of high temperature CNTs.

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## **Geometric analysis and isolation of overlapping resonances of the many open and degenerate many closed channels system studied by multichannel quantum defect theory**

이천우, 김정진

아주대 화학과

Isolation of the overlapping resonances in the photoionization spectra using multichannel quantum defect theory (MQDT) in systems involving one open channel and many degenerate closed channels system was managed in the previous study (Lee. C.-W., J. Phys. B 2010. 43, 175002). It was extended to manage the many open and degenerate many closed channels system. This theory was applied to the dipole allowed  $J = 1$  spectra for rare gas atoms Ar, Kr, Xe and group IV elements, Ge, Sn and Pb. In this time, the theory was applied to group II element Sr and transition metal element Cu.

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## **Effect of an interloper in the perturbed autoionizing Rydberg series involving four-channels system by multichannel quantum defect theory.**

이천우, 김정진

아주대 화학과

In the complex autoionization spectra which is overlapping resonances, Rydberg series that perturbed by an interloper is important system. A single lower-lying series, which separates the interloper's spectra from the autoionizing Rydberg series, was extended to a system involving two lower-lying autoionizing series. A method, Merged view system, was found to be negligible in the spectrum obtained by Kalyar et al., (2009). In the detailed method which was used formulation could be allowed spectrum of four-channel system and to be treated similar to that of three-channel system. The method was restricted in the single lower-lying series system. In this time, a study has solved the restriction that manage two lower-lying channels each thereby using a non-merged view. It provides an information of topological shifts of an interloper and perturbed system in that of the autoionizing Rydberg series.

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## Molecular dynamic simulation for cooling behavior of water: thermodynamic properties and hydrogen-bond network

최봉식, \*박승호, \*송인성, \*신동주, \*위영현, \*조철희, 이억균

KAIST 화학과 \*한국과학영재학교 화학생물학부

Water is an essential and widely populated substance for living organisms. Therefore, water is engaged in numerous vital phenomena. For instance the dynamics of biomolecules, especially proteins, is closely related to the interactions with water molecules. Interestingly, water has its unique features different from other compounds. One of them is a characteristic density maximum at 4°C, and this feature is mainly originated from its intermolecular hydrogen bond interactions. We investigated the properties of water when being cooled by computer simulation. Molecular dynamic calculation was done using the widely used MD simulation code, LAMMPS. MD simulation runs were performed under NPT ensemble with 1000 TIP4P water molecules, in conjunction with the SHAKE algorithm to keep the molecules rigid. Cooling was done on the system by using Nose-Hoover thermostat with constant cooling rate for different initial conditions. The cooling behavior of water was then studied by observing the thermodynamic and structural properties of water as initial temperature varied. While on cooling, the maximum density point appeared from the volume profile obtained from simulation. The number and the lifetimes of hydrogen bonds increased as the temperature decreased. These results can be explained on the structural transformations between open and closed H-bond networks.

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## Raman Spectroscopy Study of Graphene on Atomically Flat Boron Nitride

안광현, 고택영, 류순민

경희대 응용화학과

Graphene, a single layer of graphite, has attracted significant research interest since its first isolation from graphite. Interactions between graphene and amorphous substrate like  $\text{SiO}_2/\text{Si}$  have been shown to limit charge mobility and mediate spontaneous hole doping in the ambient conditions. In this study, we have investigated environmental and substrate-induced charge doping in graphene supported on hexagonal boron nitride, atomically flat insulating substrates. The layered composite samples were prepared by transferring mechanically exfoliated or CVD-grown graphene onto cleaved boron nitride flakes supported on  $\text{SiO}_2/\text{Si}$  substrates. Atomic force microscopy and Raman spectroscopy have been exploited to unravel the influence of atomically flat substrates on morphology and environmental charge doping in graphene.



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## Charge Transfer between Graphene and a Strong Electron Acceptor, Tetrafluorotetracyanoquinodimethane (F4-TCNQ)

이지은, \*양성익, \*이영식, 류순민

경희대 응용화학과 \*경희대 화학과

Graphene, a single atomic layer of sp<sup>2</sup>-bonded carbon, shows substantial potential for various applications. Chemical manipulation of its electronic properties will be of great importance. In this study, we have investigated interaction between graphene and organic molecular layer of tetrafluorotetracyanoquinodimethane (F4-TCNQ), a strong electron acceptor. F4-TCNQ films of varying thickness were evaporated onto graphene mechanically exfoliated on SiO<sub>2</sub>/Si substrates. F4-TCNQ molecules increase the frequencies of Raman G and 2D bands of graphene while decreasing the linewidth of G band and 2D/G intensity ratio, which is consistent with increase of hole density in graphene. These results exemplify the possibility of chemical tuning of electronic properties of graphene.

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## Morphology and Thermal Oxidation of Atomically Flat Graphene Supported on Mica

고택영, 류순민, 심지혜

경희대 응용화학과

Graphene has many fascinating material properties such as high electron mobility, high optical transparency, excellent thermal conductivity, superior Young's modulus, etc. Several studies have recently found that single-layer graphene is chemically more reactive than few-layer graphene when supported on silicon dioxide substrates with sub-nm roughness. In this study, we have investigated the influence of chemical reactivity of graphene. Morphology and thermal oxidation behavior of atomically flat mica substrates were studied by atomic force microscopy and Raman spectroscopy compared to graphene on SiO<sub>2</sub>/Si substrates. Notably, oxidation of single-layer graphene proceeds more slowly on mica than SiO<sub>2</sub>/Si. Detailed analysis led to a conclusion that deformation along the out-of-plane direction enhances reactivity of graphene.

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## Control of the nanostructure and hydrophobicity of polystyrene surfaces

홍다정, \*류일환, \*곽현태, 임상규

국민대 생명나노화학과 \*국민대 화학과

Superhydrophobic surface is attracting growing attention for a wide range of industrial applications such as the production of anti-fogging and/or self-cleaning substrates. In this work, superhydrophobic polystyrene (PS) surfaces were obtained by corrugating the surfaces in a nanometer scale. The surface nano-corrugation was performed using a simple nano-imprint technique with polydimethylsiloxane coated anodic aluminum oxide (AAO) master templates. The master templates with simple and stepped nanohole structures at various dimensions were fabricated by controlling the oxidation conditions during the process of AAO production. The alteration of the PS surface nanostructures led to the variation of water contact angle (CA) and hydrophobicity of the surfaces.

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## Characterization of chemically oxidized carbon nanotubes

공혜진, \*임상규, \*한지영

국민대 화학과 \*국민대 생명나노화학과

Carbon nanotubes (CNTs) tend to aggregate into bundles due to their nano size and high surface energy. As a result, CNTs are difficult to disperse in organic media, which hampers transferring their unique mechanical and electrical properties to the CNT-contained composites. In this context, oxidative surface functionalization of CNTs is crucial for their further applications since the grafting of chemical functionalities such as carboxylates on the CNT surface is known to increase the electrostatic stability required for a colloidal dispersion. In this work, the surface of multiwalled carbon nanotubes (MWCNTs) were chemically functionalized by strong oxidants such as nitric acid and sulfuric-nitric acid mixture (3:1) at various oxidation conditions. The extent of functionalization was determined by titration measurements, Fourier-transform infrared spectroscopy (FTIR) and x-ray photoelectron spectroscopy (XPS). Especially, the different functionalities produced during the oxidation could be quantitatively estimated by XPS. Morphological changes were also detected by scanning and transmission electron microscopy.

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## Size Dependence of Nanoscale Self Assembled Monolayers

**Saha Joyanta Kumar**, \*장준경

부산대 나노융합기술학과 \*부산대 나노정보소재공학과

We studied the properties of nanoscale self-assembled monolayers (SAMs) of alkanethiol on gold using molecular dynamics simulations. By varying the diameter of SAM from 1.4 to 3.6 nm we examined its stability, ordering in orientation, reorientation dynamics, and transport property. SAMs of 2.2 nm or more in diameter are bulk-like in that alkyl chains stand up and sulfur atoms are packed compactly. We found the tilt direction of chain of alkanethiol precessed clockwise or counterclockwise around the center of SAM. The change in the precession direction became more frequent as the SAM decreases in size. We found the precession lasted for less than 1 ns and then changed its direction. With less than 2.2 nm in diameter, the alkyl chains of SAM lie down on the surface. This indicates that the ultimate resolution of the SAM pattern achievable in soft nanolithography is 2.2 nm in width.

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## Density Functional Theory Study of catechol adhesion on Wet Silica Surface

Mian Shabeer Ahmad, \*장준경

부산대 나노융합기술학과 \*부산대 나노정보소재공학과

Catechol (1, 2-dihydroxybenzene) functionality of marine mussels is speculated to be responsible for its strong and versatile adhesion on various wet surfaces. To enlighten the features of this adhesion, we performed a periodic density functional theory calculation for catechol adsorption on silica surfaces. We obtained its binding energy and geometry on two representative hydroxylated surfaces of cristobalite, which mimic amorphous silica. Catechol strongly adhered to both surfaces by making three or four hydrogen bonds. To investigate the competitive adsorption of catechol and water on a wet silica surface, we show the spontaneity of reaction in which catechol displaces water molecules to adhere directly to the surface. This is also substantiated by our molecular dynamics simulation

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## Synthesis and luminescence properties of Eu(II)-coated SiO<sub>2</sub> nanoparticles

김종문, 정용광, 강준길, \*손영구

충남대 화학과 \*영남대 화학과

Blue europium(II) complexes with acid organophosphorous were synthesized using the Eu<sub>2</sub>O<sub>3</sub> solution. The acid organophosphorous used in this work were Bis(2-ethylhexyl)-phosphate (BEHP) and 2-ethylhexyl hydrogen 2-ethylhexyl phosphonate (EHEP). SiO<sub>2</sub> nanoparticles were prepared using a TEOS precursor and then the nanoparticles were coated with Eu(II) complexes. The photophysical properties of Eu(II)-coated SiO<sub>2</sub> nanoparticles were investigated in terms of excitation, luminescence, decay time and quantum yield.

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## Promotional effect of hydrogen peroxide for water splitting over anatase TiO<sub>2</sub> nanosheets

공자현, \*김유권

아주대 에너지 시스템학부 \*아주대 자연과학부

TiO<sub>2</sub> is known to be a promising photocatalyst for splitting water into hydrogen and oxygen. In this study, we prepared anatase TiO<sub>2</sub> nanocrystals for a photocatalytic activity measurement in an aqueous solution. For comparison, we compare the photocatalytic activity of our anatase TiO<sub>2</sub> and commercial P-25. We also examine a promotional effect of hydrogen peroxide in photocatalytic water splitting on our TiO<sub>2</sub> nanocrystals. Combined measurements of GC and Infrared spectroscopy are employed to propose involved water splitting reaction mechanism.



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## Adsorption Patterns of Gold Nanoparticles on Methyl-Terminated Self-Assembled Monolayers

이성운, 윤상운

단국대 화학과

Understanding the adsorption of gold nanoparticles (AuNPs) on self-assembled monolayers (SAMs) is important because an assembly of the AuNPs-SAM-gold substrate provides easily controllable metal-metal junctions, in which fascinating phenomena such as electron tunneling and surface-enhanced Raman scattering can occur. In this article, we report strikingly different adsorption patterns of AuNPs on methyl-terminated SAMs. In contrast to the general belief that the terminal functional groups determine the surface properties of SAMs, the AuNPs adsorb on the surfaces of SAMs of methylbenzenethiol (MBT) SAMs in a uniform, dispersed fashion, whereas aggregated adsorption is observed on the surfaces of SAMs of alkanethiols. We explore the effects of the terminal methyl group orientation, structural properties of SAMs, such as orderliness and packing density, and surface energies on the adsorption pattern differences. Dispersed or aggregated adsorption is determined by whether the citrate anions on the AuNPs are retained or removed by the SAM surfaces during the adsorption and thus, is critically dependent on the extent of the interactions between the AuNPs and SAMs. Direct interactions between the AuNPs and hydrophobic surfaces of alkanethiol SAMs strip the AuNPs of their citrate layers, leading to aggregated adsorption. For the less hydrophobic MBT SAMs, water mediates and softens the adsorption of the AuNPs. As a result, the citrate anions are retained on the AuNP surfaces, leading to dispersed adsorption of AuNPs. Forced interactions between the AuNPs and the MBT SAM surfaces by vigorous stirring yield aggregated adsorption, supporting our model.

일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: III-PHYS.P-139

발표분야: 물리화학

발표종류: 포스터, 발표일시: 금 10:30~12:30

## Protective Coatings on Sulfide- and Selenosulfide-based Phosphors and their Luminescence

강봉호, 정용광, 강준길

충남대 화학과

Sulfide- and selenosulfide-based phosphors were coated with metal oxides ( $\text{SiO}_2$ ,  $\text{Al}_2\text{O}_3$ , and  $\text{MgO}$ ), organic compounds (silane, malenic anhydride, PEG, polystyrene, and polymethyl methacrylate) and metal oxide-organic hybrides. The luminescence intensities of uncoated and coated phosphors were measured at several high temperatures. Furthermore, uncoated and coated phosphors were fabricated with 7-chip B-LEDs and their luminescence properties were investigated under high temperature and moisture condition.

일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: III-PHYS.P-140

발표분야: 물리화학

발표종류: 포스터, 발표일시: 금 10:30~12:30

## Interaction of $\text{NH}_3$ with $\text{TiO}_2$ nanocrystals at elevated substrate temperatures

신동희, \*김유권

아주대 에너지시스템학부 \*아주대 자연과학부

Nitrogen doping into  $\text{TiO}_2$  is a promising way of improving photocatalytic activity. In this study,  $\text{NH}_3$  is employed as a source of nitrogen and we study the kinetics of nitrogen doping into a nanocrystalline  $\text{TiO}_2$  powder using a systematic measurement of reaction products using GC.  $\text{NH}_3$  interaction with  $\text{TiO}_2$  surface is found to produce  $\text{H}_2\text{O}$  and  $\text{NO}$  as a reaction product at the substrate temperature lower than 500 K. We propose a possible reaction mechanism based on our measurements.

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발표코드: III-PHYS.P-141

발표분야: 물리화학

발표종류: 포스터, 발표일시: 금 10:30~12:30

## Characterization of Re(III) complexes for white LED (Re = Sm, Eu, Tb and Dy)

장지아, 정용광, 강준길

충남대 화학과

The complexes of  $[\text{Re}(\beta\text{-diketone})_4]^-$ ,  $[\text{Re}(\beta\text{-diketone})_3(\text{phen})]$  and  $[\text{Re}(\text{phen})_2(\text{NO}_3)_3]$  (Re = Sm, Eu, Tb and Dy) were synthesized and their photophysical properties were investigated. The  $\beta$ -diketones used in this work were acetylacetone, 4,4,4-trifluoro-1-(2-furyl)-1,3-butanedione, 4,4,4-Trifluoro-1-(2-naphthyl)-1,3-butanedione and dibenzoylmethane. The complexes excited at UV produced sensitized visible luminescence and their luminescence efficiencies were determined. In this presentation, not only the energy transfer from a sensitizer to Re(III) but also the incorporation of the complex with  $\text{SiO}_2$  nanoparticle will be precisely discussed.

일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: III-PHYS.P-142

발표분야: 물리화학

발표종류: 포스터, 발표일시: 금 10:30~12:30

## Size-controllable synthesis of silver nanoparticles and their plasmonic effect.

김민아, 강준길, \*손영구

충남대 화학과 \*영남대 화학과

Silver nano particles with a few nanometer size were synthesized using HDEHP (Bis(2-ethylhexyl)phosphate) and PC88A(Mono(2-ethylhexyl) 2-ethylhexylphosphonate) as dispersing reagents. It was found that the size and uniformity of silver particles were dependent on the reaction parameters, such as the concentrations of  $\text{AgNO}_3$ , the dispersing reagent and hydrazine. Silver nanoparticles with the size of 2 - 20nm was obtained controllably by tuning the reaction parameters,. Furthermore, the interaction of silver nanoparticles with 1,10-phenanthroline were monitored by absorption and luminescence time-profiles. With increasing the reaction time, the localized surface plasmon resonance (LSPR) effect increased. The LSPR effect due to 1,10-phenanthroline was visualized by TEM.

일시: 2011년 4월 28~29일(목~금) 2일간

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발표코드: III-PHYS.P-143

발표분야: 물리화학

발표종류: 포스터, 발표일시: 금 10:30~12:30

## UV-UV hole burn spectroscopy of an isolated dibenzo-18-crown-6-ether complex with a potassium cation

최대호, 최창민, 김남준

충북대 화학과

We have developed a method to obtain a UV-UV hole burn spectrum in a quadrupole ion-trap reflectron time-of-flight mass spectrometer. Different from the case of a neutral molecule, the separation of the ions produced by the hole burn laser from those by the probe laser is nearly impossible for ions stored in the ion trap. We found that the separation is possible if we detect the direct fragment ions ejecting out of the ion trap as soon as we irradiated the laser pulse onto the ions in the ion trap. The fragment ions by the hole burn laser are detected earlier than those by the probe in the time-of-flight mass spectrometer, which is attached to the ion trap. This technique is tested by obtaining the UV-UV hole burn spectrum of an isolated dibenzo-18-crown-6-ether complex with a potassium cation.

일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: III-PHYS.P-144

발표분야: 물리화학

발표종류: 포스터, 발표일시: 금 10:30~12:30

## Synthesis and photo-luminescence properties of bright yellowish green emitting phosphor

정용광, 장지아, 강준길

충남대 화학과

Eu<sup>2+</sup>-doped MtSrxSiyNz (M = divalent or trivalent metal ions) phosphors were synthesized through hydrothermal method and ammonia nitridation method. First, SrxSiyNz was prepared in liquid ammonia, following by thermal treatment. Second, the initial materials, SrxSiyNz, MmNn and Eu<sub>2</sub>O<sub>3</sub> were taken in stoichiometric properties. The mixture was fired at 1400 – 1500 °C for 4 h under NH<sub>3</sub> gas. then was treated at mixed with Eu<sub>2</sub>O<sub>3</sub> and some metal nitrides. Morphology and photophysical properties of MtSrxSiyNz:Eu<sup>2+</sup> were characterized by FE-SEM, XRD and luminescence spectroscopy. It was found that Eu<sup>2+</sup> doped (Zn<sub>3</sub>SrSi<sub>2</sub>)<sub>3</sub>N<sub>16</sub> phosphor excited at blue light produced strong yellowish green emission. Furthermore, the prepared phosphors were casted on blue LEDs and their luminescence properties were investigated.

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장소: 제주ICC

발표코드: III-PHYS.P-145

발표분야: 물리화학

발표종류: 포스터, 발표일시: 금 10:30~12:30

## Synthesis and Luminescence Properties of Red Nitride phosphors

장지아, 정용광, 강준길

충남대 화학과

Red nitride phosphors,  $\text{CaSrM}_x\text{Si}_y\text{N}_z:\text{Eu}^{2+}, \text{Re}^{3+}$  ( $M = \text{B}$  or  $\text{Ga}$ ,  $\text{Re} = \text{rare earth}$ ), were synthesized by ammonia nitridation and solid state reaction methods. First,  $\text{Sr}_x\text{Si}_y\text{N}_z$  was prepared in liquid ammonia, following by thermal treatment. Next,  $\text{Sr}_x\text{Si}_y$  was mixed with the materials,  $\text{M}_m\text{N}_n$ ,  $\text{Eu}_2\text{O}_3$  and  $\text{Re}_2\text{O}_3$  in stoichiometric properties. The mixture metals were heated at 1400-1500 °C for 6 h under  $\text{NH}_3$  condition. The prepared phosphors were characterized by FE-SEM, XRD and luminescence spectroscopy. The phosphors, excited at 460 nm, produced the red emission spanned over 580 – 730 nm.



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발표코드: III-PHYS.P-146

발표분야: 물리화학

발표종류: 포스터, 발표일시: 금 10:30~12:30

## **Mg<sup>2+</sup>-exchanged Zeolites Y (FAU, Si/Al=1.56) and its single-crystal structure**

**김후식, 서성만, \*김경화, 고성운, 이오석, 임우택**

안동대 응용화학과 \*포항가속기연구소 빔라인부 엑스선운영2팀

The Single-crystal of Mg<sup>2+</sup>-exchanged zeolite Y was prepared by dynamic (flow) ion exchange with 0.05 M MgCl<sub>2</sub>·6H<sub>2</sub>O aqueous solution at 293K for 3days, followed by dehydration at 673 K and 1 x 10<sup>-6</sup> Torr for 2days. The Single-crystal of Mg<sup>2+</sup>-exchanged Zeolite Y, [Mg<sub>39</sub>][Si<sub>100</sub>Al<sub>75</sub>O<sub>384</sub>]-FAU per unit cell (*a* = 24.5060(1) Å) was determined by single-crystal X-ray diffraction techniques in the cubic space groups *Fd3-m* at 100 K. The structure was refined using all intensities to the final error indices (using only the 561 reflections for which *F<sub>o</sub>* > 4(*F<sub>o</sub>*)) *R*<sub>1</sub> = 0.0386 (based on *F*) and *R*<sub>2</sub> = 0.1083 (based on *F*<sup>2</sup>). About thirty-nine Mg<sup>2+</sup> ions per unit cell are found at four different crystallographic sites. The 14 Mg<sup>2+</sup> ions occupied at site I, at the centers of double 6-ring (D6Rs, Mg-O = 2.231(3) Å and O-Mg-O = 89.1(1) and 90.9(1)°). The 3 Mg<sup>2+</sup> ions are found at site I' in the sodalite cavity opposite D6Rs (Mg-O = 2.22(3) Å and O-Mg-O = 91.7(13)°), each coordinates to a OH<sup>-</sup> ion. The 22 Mg<sup>2+</sup>ions fill at two nonequivalent positions of sites II (in the supercage) with occupancies 17 and 5 ions, respectively, (Mg-O = 2.126(4), 2.195(6) Å and O-Mg-O = 119.5(3), 113.5(4)°).

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발표분야: 물리화학

발표종류: 포스터, 발표일시: 금 10:30~12:30

## Crystallographic Studies of Mesitylene Sorption Complex of Fully Dehydrated Fully $\text{Mn}^{2+}$ -exchanged Zeolite Y (FAU)

Md. Shamsuzzoha, 서성만, \*김영훈, 임우택

안동대 응용화학과 \*안동대 환경공학과

The structure of mesitylene sorption complex into fully dehydrated fully  $\text{Mn}^{2+}$ -exchanged Zeolite Y, ( $[\text{Mn}_{37.5}][\text{Si}_{117}\text{Al}_{75}\text{O}_{384}]\text{-FAU}$ ,  $\text{Si/Al} = 1.56$ ) was determined by single crystal X-ray diffraction techniques using synchrotron radiation in the space group  $Fd\bar{3}m$  at 100(1) K. The sorption crystal was prepared at 297(1) K for 3 days by treating zeolitically dried mesitylene. The dark-brown crystal was appeared. The structure was refined using all intensities to the final error indices (using the 570 reflections for which  $F_o > 4\sigma(F_o)$  of  $R_1 = 0.063$  (based on  $F$ ) and  $wR_2 = 0.151$  (based on  $F^2$ ). All of 37.5  $\text{Mn}^{2+}$  ions are occupied at four equipoints ; 14.5 and 3  $\text{Mn}^{2+}$  ions are found at the centers of the double 6-rings (site I) and in the sodalite cavity, respectively. The remaining 20  $\text{Mn}^{2+}$  ions are located in the supercage near single 6-rings at two nonequivalent sites II with occupancies of 5 and 15  $\text{Mn}^{2+}$  ions. Fifteen mesitylene molecules lie on 3-fold axes in the supercage where they interact facially with the 15  $\text{Mn}^{2+}$  ions at site II. The  $\text{Mn}^{2+}$  ions at site II extend more *ca.* 0.42 Å inside the supercage from the plane of the three oxygens to which it is bound compared with  $\text{Mn}_{37.5}\text{-Y}$ . The hydrogen atoms of methyl groups of mesitylene are near framework oxygens and interact with these oxygens by electrostatic and van der Waals forces. Sorbed mesitylene molecules appear to be distorted in the same way.

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발표코드: III-PHYS.P-148

발표분야: 물리화학

발표종류: 포스터, 발표일시: 금 10:30~12:30

## Investigation of a Single Crystal Structure of *m*-xylene Sorption Complex of Fully Dehydrated Fully Mn<sup>2+</sup>-exchanged Zeolite Y (FAU)

Md. Shamsuzzoha, 최식영, 임우택

안동대 응용화학과

The single-crystal structure of *m*-xylene sorption complex of fully dehydrated fully Mn<sup>2+</sup>-exchanged Zeolite Y, [Mn<sub>37.5</sub>(C<sub>8</sub>H<sub>10</sub>)<sub>19</sub>][Si<sub>117</sub>Al<sub>75</sub>O<sub>384</sub>]-FAU, was determined by single-crystal synchrotron X-ray diffraction techniques using 0.90000 Å-wavelength radiation in the space group *Fd3-m* at 100(1) K and refined using all intensities to the final error indices (using the 565 reflections for which  $F_o > 4\sigma(F_o)$ ) of  $R_1 = 0.081$  (based on  $F$ ) and  $wR_2 = 0.216$  (based on  $F^2$ ). The sorption crystal was prepared at 297(1) K for 3 days by treating zeolitically dried *m*-xylene and black crystal was observed. In this structure, there are four crystallographic sites for all 37.5 Mn<sup>2+</sup> ions; 14.5 Mn<sup>2+</sup> ions are occupied at the centers of the double 6-rings (site I). Filling site I' and site II' in the sodalite cavity are 2 and 2 Mn<sup>2+</sup> ions, respectively. The remaining 19 Mn<sup>2+</sup> ions are located in the supercage near single 6-rings at site II. Nineteen *m*-xylene molecules lie on 3-fold axes and interact facially with the 19 Mn<sup>2+</sup> ions at sites II. The Mn<sup>2+</sup> ions at site II extend more *ca.* 0.49 Å inside the supercage from the plane of the three oxygens to which it is bound compared with Mn<sub>37.5</sub>-Y. Methyl groups are displaced from their plane to the framework. The distances of hydrogen atoms of methyl groups are H...O = 2.78 and 3.09 Å and there are little electrostatic and van der Waals forces.

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장소: 제주ICC

발표코드: III-PHYS.P-149

발표분야: 물리화학

발표종류: 포스터, 발표일시: 금 10:30~12:30

## Conversions of carbon dioxide to formic acid on the B<sub>N</sub>-BNNT sidewall

최희철, 박영춘, 이윤섭

KAIST 화학과

A sufficient supply of energy is one of the most important challenges for the future of human society. Among the various known energy carriers, hydrogen could play an important role. One of the major obstacles to use hydrogen for energy applications however, is the efficient storage and handling of hydrogen. To obtain a balanced gravimetric and volumetric hydrogen storage density, pure hydrogen can be stored in compressed gaseous or liquid form and adsorbed on porous materials, e.g. zeolites or metal organic frameworks. In addition, due to the high mass amount of hydrogen in organic molecules, i.e. methanol and formic acid, these materials are feasible storage media. Especially, storage of hydrogen in formic acid (HCOOH) has the advantage of a low reaction enthalpy ( $\Delta H_{298K} = 14.7$  kJ/mol)[1] for the hydrogenation/dehydrogenation of CO<sub>2</sub>. In our previous work[2], it was shown that boron-rich boron nitride nanotube (BNNT) could capture CO<sub>2</sub> effectively at ambient conditions with the ab initio calculation results that the CO<sub>2</sub> chemisorption energy on boron antisite (B<sub>N</sub>) in BNNT is almost independent of tube diameter and higher than the standard free energy of gaseous CO<sub>2</sub> at room temperature. We have investigated the potential of utilizing the CO<sub>2</sub>-adhesive BN defect as a catalyst for the CO<sub>2</sub> conversion to HCOOH. In this work, we suggest the mechanism of CO<sub>2</sub> conversion to HCOOH by applying ONIOM(wB97X-D/6-31G\*\*):AM1 level of theory. ※ References[1] National Institute of Standards and Technology, Database 101, 2006, rel. 14.[2] Choi, H.; Park, Y. C.; Kim, Y.-H.; Lee, Y. S. *J. Am. Chem. Soc.* 2011, 133, 2084.

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발표코드: III-PHYS.P-150

발표분야: 물리화학

발표종류: 포스터, 발표일시: 금 10:30~12:30

**Determination of Si/Al Ratio of Synthetic Na-Analcime by Single-crystal X-ray Diffraction Technique and Its Single-crystal Structure,  
[Na<sub>0.94</sub>(H<sub>2</sub>O)][Si<sub>2.06</sub>Al<sub>0.94</sub>O<sub>6</sub>]-ANA**

서성만, 김후식, 고성운, \*김경화, 임우택

안동대 응용화학과 \*포항가속기연구소 빔라인부 엑스선운영2팀

Large colorless single crystals of analcime with diameters up to 0.20 mm have been synthesized from gels with the composition of 3.00SiO<sub>2</sub> : 1.50NaAlO<sub>2</sub> : 8.02NaOH : 454H<sub>2</sub>O : 5.00TEA. The fully Na<sup>+</sup>-exchanged analcime have been prepared with aqueous 0.1 M NaCl (pH adjusted from 6 to 11 by dropwise addition of NaOH). The single-crystal structure of hydrated [Na<sub>0.94</sub>(H<sub>2</sub>O)][Si<sub>2.06</sub>Al<sub>0.94</sub>O<sub>6</sub>]-ANA per unit cell,  $a = 13.703(3)$  Å has been determined by single-crystal X-ray diffraction technique in the orthorhombic space group  $I_{bca}$  at 294 K. The structure was refined using all intensities to the final error indices (using only the 1,446 reflections for which  $F_o > 4\sigma(F_o)$ )  $R_1/R_2 = 0.054/0.143$ . About 15 Na<sup>+</sup> ions are located at three nonequivalent positions and octahedrally coordinated. The chemical composition is Na<sub>0.94</sub>(H<sub>2</sub>O)Si<sub>2.06</sub>Al<sub>0.94</sub>O<sub>6</sub>. The Si/Al ratio of synthetic analcime is 2.19 determined by the occupations of cations, 14.79, in the single-crystal determination work.

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장소: 제주ICC

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발표분야: 물리화학

발표종류: 포스터, 발표일시: 금 10:30~12:30

## Universal Dynamic Phase Transition in Reaction Event Counting Statistics of Dynamically Heterogeneous Single Molecules with Slow Conformational Dynamics

임유림, 성재영

중앙대 화학과

Reactivity fluctuations of single molecules are ubiquitous, and their effects manifested on a series of reaction times of single molecule systems are directly observable with the advance of single molecule experimental techniques. At this point, an important new theoretical challenge is to extract meaningful information from the fluctuating reaction time series of single molecule systems. While a few research efforts have been directed toward quantitative interpretation of statistical distribution of individual reaction times of single molecule systems, the significance of reaction event counting statistics as a valuable single molecule experimental observable is yet to be recognized for most single biomolecule systems. In this paper, we first report a universal dynamic phase transition in reaction number fluctuation of a single biomolecule system, which directly provides information about reaction coupled, slow conformational dynamics of the biomolecules. Meanwhile, we present novel single molecule experimental observables that allow separate quantification of the fluctuation resulting from heterogeneity between different single molecules and that resulting from intrinsically stochastic nature of chemical reactions persistent even in a homogenous single molecule system. We find that the fluctuation proportional to the square of the mean reaction number results from the heterogeneous reactivity of molecular system and it can be dominant at short times; in comparison, the fluctuation linearly proportional to the mean reaction number prevails at long times at which the reactivity difference between individual molecules can be neglected.

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발표코드: III-PHYS.P-152

발표분야: 물리화학

발표종류: 포스터, 발표일시: 금 10:30~12:30

## **SPOT-synthesis data provides information on SH3-domain-mediated complex formation**

한승수

KAIST 바이오및뇌공학과

The SH3 domain is a common protein interaction domain involved in various biological processes and typically binds to proline-rich regions in proteins. SH3 domains recognize their partners via a weak, transient interaction and, therefore, are promiscuous in nature. However, many computational models assume that this domain forms a stable complex. To explain the real binding property of the SH3 domain-ligand complex, we proposed a physical model (MS model) and applied the model to semi-quantitative binding affinity data from SPOT synthesis (positionally addressable synthesis of peptides on continuous cellulose membrane supports). The results showed not only that our MS model describes SPOT-synthesis data better than a conventional model, but also that the model provides a correlation to the dissociation constants better than directly using the SPOT data. Localization analysis based on our model shows that SH3 domains make complexes with many proteins by binding at several sites, which are proximally located in the proteins, as well as by binding a specific site. Importantly, this result suggests that, for achieving appropriate biological function, proteins have evolved a part of their sequence which recognizes SH3 domains toward two different directions: providing a specific sequence site for a tight binding or providing multiple sites for higher population of the complex with keeping a higher exchange rate between the free and bound states.

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발표분야: 물리화학

발표종류: 포스터, 발표일시: 금 10:30~12:30

## Surface Plasmon Enhanced Photoconductance in Mesoporous TiO<sub>2</sub> Nanofibers Loaded with Au Nanoparticles

임지은, 오승임, 김용록

연세대 화학과

We synthesized mesoporous TiO<sub>2</sub> nanofibers loaded with Au nanoparticles (MTNF-Au) and investigated the influence of surface plasmon resonance (SPR) on the conductivity. MTNF-Au single nanofiber-based devices were fabricated and their plasmon-induced photocurrents were measured under visible light. In addition, we also carried out low temperature transport measurements to investigate the effects of Au nanoparticles on the electronic transport properties. This study shows that utilization of surface plasmon resonance of Au nanoparticles can be a method for improvement of the photoconversion efficiency of solar cell.



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## Target oriented Photofunctional Magnetic Nanoparticles

민정명, 왕강균, 김혜리, 김용록

연세대 화학과

자성나노입자는 MRI 조영제, 약물 전달체등의 의학적 이용뿐만 아니라 유해성 환경 검출 및 분해의 기본물질로 널리 응용 되어진다. 최근 이러한 자성나노입자에 다양한 유/무기 물질을 도입한 다기능성 자성나노입자의 제조 및 이의 응용에 대해 많이 연구 되어지고 있다. 본 연구에서는 자성나노입자에 활성산소 생성 유기물과 특정 생체물질에 선택적 결합을 유도하는 생유기물이 도입된 복합 기능성 자성나노입자를 제조하였다. 제조된 복합기능성 자성나노물질은 주사전자 현미경(SEM)과 투과전자 현미경(TEM)을 이용해 형상을 확인하였으며, 정류 상태 분광법(UV-Vis, Fluorespectroscopy, FT-IR)을 이용하여 광물리적 특성을 규명하였다. 또한 시분해 레이저 분광법을 이용하여 제조된 복합기능성 자성나노입자로부터 생성되는 단일항 산소를 직접적으로 측정하고, 간접적 방법인 광촉매 반응을 이용하여 생성된 활성산소의 종을 확인하였다. 제조된 복합기능성 자성나노입자는 생성되는 활성산소를 이용하여 다양한 바이러스, 박테리아 등 유해성 생체물질을 분해할 수 있어 의료 또는 환경 분야 등에 널리 응용 되어질 것으로 기대된다.

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## Detection of Estrogen Hormone with Electrochemical Impedance Spectroscopy by Immobilized Estrogen Receptor on Au Electrode

LIJING, 임지은, 김병건, 이원용, 김용록

연세대 화학과

Immunobiosensor for the electrochemical detection of estrogen hormone (17-estradiol) was developed by using an estrogen receptor alpha (ER- $\alpha$ ) immobilized onto the gold electrode. It was fabricated by stepwise immobilization of the cross linkers and ER- $\alpha$ . Binding of 17-estradiol to the electrode increased the electron-transfer resistance, which was directly detected by electrochemical impedance spectroscopy (EIS). 17-estradiol was successfully detected with the concentration range of  $10^{-9}$ ~ $10^{-13}$  M. The affinity between 17-estradiol and the immobilized ER- $\alpha$  was estimated to be 0.0455 M<sup>-1</sup>. The electrochemical biosensor fabricated in this study successfully demonstrates ultra-high sensitivity and selectivity for the detection of 17-estradiol.

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## Photo-functional Polymer Matrix for Elimination of Bio-hazardable Systems

김수진, 왕강균, 정지혜, 오승임, 김용록

연세대 화학과

최근 활성산소의 높은 활성능력을 이용한 유해성물질의 제거에 대한 연구가 활발히 진행되어지고 있다. 특히 의학, 환경 분야의 일부에서는 활성산소를 이용한 높은 효율성의 유해성 생체물질 제거시스템들에 대한 상용화연구가 많이 진행 되고 있다. 그중 실리콘 폴리머는 현재 의료용 기구, 환경 분야 등에 폭넓게 사용되어지고 있으나 박테리아, 바이러스 등의 세균흡착에 의해 쉽게 오염되는 문제점이 있다. 따라서 본 연구에서는 실리콘 폴리머에 가시광 영역에서 높은 흡광률을 갖는 광감응분자를 도입하여 광기능성 폴리머 소재를 제조하고, 제조된 물질의 구조와 형상 및 광 물리적 특성을 공초점 현미경, 주사전자현미경, 정류상태 흡수-형광분광법등을 이용하여 규명하였다. 또한 시간-파장분해 단일항 산소 인광 분광법을 이용하여 광기능성 폴리머 소재에서 생성되는 단일항 산소를 직접적으로 검출하고, 생성되는 활성산소를 광촉매 실험을 통해 활성산소의 활성특성을 연구하였다. 더 나아가 응용가능성을 검증하기 위하여 유해성 세균주를 대상으로 멸균효능을 검증하였다.

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## **Fabrication and performance of photofunctional magnetic nanoparticles for the elimination of environmental hazard materials.**

신언필, 최경훈, 오승임, \*황정옥, 김용록

연세대 화학과 \*연세대 이과대학 화학과

We report a novel photofunctional magnetic nanoparticle that is strategically designed and prepared by simple modification process. Photofunctionality is provided by the photosensitizer (PS) that generates singlet oxygen in high quantum yield. The PS molecules are covalently bonded to the surface of magnetic nanoparticle. Microstructure and magnetic and photophysical properties of the photofunctional magnetic nanoparticles are investigated by transmission electron microscopy, vibrating sample magnetometry, and time-resolved spectroscopic methods. The results show that the immobilized PS molecules retain their optical and functional properties including the high efficiency of singlet oxygen generation. Generation quantum yield ( $\Phi\Delta$ ) and releasing yield (hD) of singlet oxygen from the prepared photofunctional magnetic nanoparticles are 0.47 and 0.42 respectively. Furthermore, the photofunctional magnetic nanoparticles have good solubility and stability in water, which are induced by the surface modification process. Photocatalytic experiment is demonstrated by utilizing the oxidation reaction of environmental hazards materials with the photofunctional magnetic nanoparticles.

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## Photofunctional Metal Alloy for Elimination of Health Hazard Materials

왕강균, 김봉진, 최경훈, 김용록

연세대 화학과

Photodynamic Therapy (PDT) is a promising approach for killing microorganism and especially for the inactivation of antibiotic-resistant strains. The photodynamic process rapidly generates reactive oxygen species (ROS) as for instance peroxides, hydroxyl radicals, superoxide ions, and singlet oxygen. Among them, the singlet oxygen is considered to be a major causative agent of cellular damage in photodynamic process. Due to advantage of the cytotoxic effect of PDT on bacteria, the PDT method has been one of the most appropriate tools to prevent the microbes which result in biofilm formation. This work describes a method of singlet oxygen generating photosensitizer (PS) coating on metal alloy which shows a good biocompatibility. The PS coated on metal alloy was prepared in one step. The photosensitizer (PS) with carboxyl group was chemically attached to the surface of metal plate by esterification method. Fabricated photofunctional metal alloy was confirmed with FT-IR, reflectance UV-Vis absorption and spectrofluorometer. The singlet oxygen generation efficiency of the photofunctional metal alloy plate was detected by an indirect chemical method by using the decomposition of 1,3-diphenyl-isobenzofuran (DPBF).

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## Identifying and reducing error in cluster expansion approximations of protein energies

한승수

KAIST 바이오및뇌공학과

Protein design involves searching a vast space for sequences that are compatible with a defined structure. This can pose significant computational challenges. Cluster expansion is a computational technique that can significantly accelerate the evaluation of protein energies by generating a simple functional relationship between sequence and energy. The method consists of several steps. First, for a given protein fold, a training set of sequences with known energies is generated. Next, this training set is used to expand energy as a function of clusters consisting of single residues, residue pairs, and higher order terms, if required. The accuracy of the sequence-based expansion is monitored and improved using cross-validation testing and iterative inclusion of additional clusters. As a trade-off for evaluation speed, the cluster-expansion approximation causes prediction errors, which can be reduced by including more training sequences, including higher-order terms in the expansion, and/or reducing the sequence space described by the cluster expansion. This paper analyzes the sources of error and introduces a method whereby accuracy can be improved by judiciously reducing the described sequence space. The method is applied to describe the sequence-stability relationship for several protein structures: coiled-coil dimers and trimers, a PDZ domain, and T4 lysozyme as examples with computationally derived energies, and SH3 domains in amphiphysin-1 and endophilin-1 as examples where the expanded pseudo-energies are obtained from experiments. Our open-source software package CLEVER allows users to expand their own energy function of interest and thereby apply cluster expansion to custom problems in protein design.

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## Synthesis of water-soluble Cerium ion doped Lanthanum fluoride nanoparticles

배연주, \*엄영랑, \*\*전지현, 김재우

한국원자력연구원 원자력재료개발부 \*한국원자력연구소 원자력재료개발부 \*\*한국원자력연구소 원자력 재료개발부

Water-soluble lanthanide ion ( $\text{Ce}^{3+}$ ) doped Lanthanum halide nanoparticles were synthesized using a simple method carried out in methanol at low temperature. The cerium ion doped lanthanum fluoride ( $\text{LaF}_3:\text{Ce}^{3+}$ ) was characterized by UV-vis spectroscopy, transmission electron microscopy (TEM), X-ray diffraction (XRD), fourier transform infrared (FT-IR) and fluorescence spectroscopy. The  $\text{LaF}_3:\text{Ce}^{3+}$  nanoparticles have a spherical shape and an average size of about 20 nm. According to excitation and emission spectra, cerium ion was doped into the  $\text{LaF}_3$  nanoparticles which showed the luminescence corresponds to electronic transitions of the  $\text{Ce}^{3+}$  ion.

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## Fabrication of three-dimensional network-structured CNTs by plasma enhanced CVD

여해구, 서정은, \*노태용, 조석진, \*\*조용덕, 이해원

한양대 화학과 \*한양대 나노과학기술연구소 \*\*한양대 나노융합과학과

Carbon nanotubes (CNTs) have attracted much attention because of their excellent electrical and mechanical properties. Especially, it is expected that an increase of surface area of CNTs can be useful for many applications such as highly sensitive electrical detectors, and optical absorbers and emitters. In order to increase the surface area of CNTs, we focused on the fabrication of high density Single-walled CNT(SWCNT) network structures on the three-dimensionally patterned substrate by both thermal chemical vapor deposition (CVD) and plasma enhanced CVD(PECVD). In the case of PECVD, the plasma decomposes hydrocarbon gases such as  $C_2H_2$ ,  $CH_4$  and  $C_2H_4$  etc. Thus, the PECVD is possible to synthesize CNTs at low temperature compared with the conventional thermal CVD process. However, the fabrication of three-dimensional network-structured SWCNTs by PECVD have many structural defects and bent structures compared to those prepared by the thermal CVD process due to a etching effect of the plasma ions. In order to fabricate three-dimensional network-structured SWCNTs by PECVD, it is necessary to reduce the plasma etching effect. In this study, a mesh-structured shield was introduced between plasma source and substrate to reduce the etching effect, and then we obtained well-distributed three-dimensional network-structured SWCNTs by PECVD.



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## **Laser-induced breakdown spectroscopy of natural salts: Quantification and discrimination**

이용훈

목포대 화학과

Laser-induced breakdown spectroscopy (LIBS) was applied to fast quantification and discrimination methods for natural salts. Laser-induced plasmas were generated by focusing a pulsed Nd:YAG laser beam. The plasma emission was collected and dispersed by a Czerny-Turner spectrometer installed with intensified charge-coupled device. The homogeneity of samples was improved by using filter paper substrates. The aqueous solutions of natural salts were absorbed into filter papers. The cyanide radical emission bands originate from carbons in paper cellulose were employed to normalize the spectral intensity. The K I, Mg I, Ca II, and Al I emission lines were simultaneously observed in LIBS spectra around 780 nm. Also, the LIBS spectra of natural salts were analyzed by multivariate statistics in order for classification and discrimination.

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## ESI-MS studies of the metal-flavonoid complexes

오가연, 최지수, 김호태

금오공과대 응용화학과

Flavonoid 화합물은 모든 질병의 원인이 되는 생체 내 산화작용을 억제한다. 산소라디칼 및 과산화지질 라디칼로부터 피부세포가 공격당하는 것을 억제하고, 금속과 결합한 화합물 역시 큰 항암작용과 항산화 작용을 가진다. Flavonoid 물질의 하나인 Quercetin 물질을 중심으로 연구를 진행하였다. Quercetin 은 가능한 세 가지 결합자리에서 경쟁 반응할 수 있는 화합물로서 3-hydroxy-and 5-hydroxy-4-carbonyl group 과 3'4'-dihydroxyl group 을 갖고 있는데, 알루미늄(III)-quercetin 착물이나 아연(II)-quercetin 착물의 항산화 효과가 quercetin 의 항산화 효과보다 증가한다고 알려져 있다. 이에 quercetin 을 중심으로 연관 물질의 metal-flavonoid 화합물 구조를 Electrospray ionization MS, MS/MS 방법으로 연구하였다.

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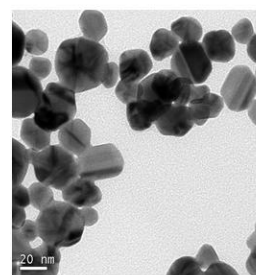
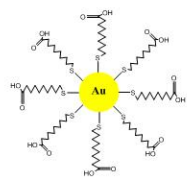
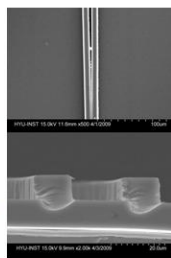
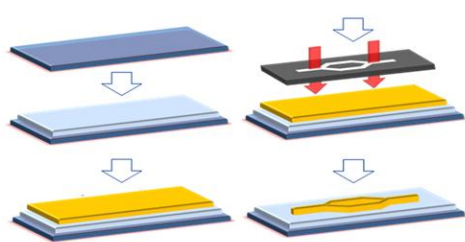
발표종류: 포스터, 발표일시: 금 10:30~12:30

## **A Simple Method for Fabricating a Mach-Zehnder Type Waveguide Using Sol-Gel Derived Photopatternable Hybrid Materials and Synthesis of Functionalized Gold Nanoparticles for Optical Biosensors**

령티빛, 형은수, 김낙중

한양대 화학과

In this work, we report on a simple method to fabricate a Mach-Zehnder type waveguide pattern using photopatternable sol-gel organic-inorganic hybrid materials. The refractive indices and propagation losses of the gel films were measured using the prism coupling method. The refractive indices of the resulting films were significantly influenced by the 3-trimethoxysilylpropylmethacrylate (TMSPM) concentration, and the average propagation loss was 0.32-0.52 dB/cm at the wavelength of 632.8 nm. The waveguides were fabricated using spin-coating and a photolithography technique. The Y-branch and straight pattern of the Mach-Zehnder waveguide were well-defined and had high transparency (>97%) in the visible region. The average thickness of the gel films was 10  $\mu\text{m}$ , and the average width of the Mach-Zehnder pattern was 10  $\mu\text{m}$ . The structural and optical properties of the fabricated patterns were analyzed using scanning electron microscopy (SEM), atomic force microscopy (AFM), near-infrared (IR) spectroscopy, and ultraviolet (UV)-visible spectroscopy. We also directly synthesized functionalized Gold nanoparticles (AuNP) using Bunte salts as ligand precursor. Here in this work, 10-Bromodecanoic acid (10-BDA) was used as a precursor of Bunte salt, and this synthesis produces functionalized AuNPs ranging from 10 to 30 nm in diameter because they are useful for sensing and biomedical applications.



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## **A complete dipeptide library reveals intrinsic backbone conformational propensities**

오광임, 조민행

고려대 화학과

Despite prolonged scientific efforts to elucidate the intrinsic peptide backbone preferences of amino acids based on understanding of intermolecular forces, many open questions remain, particularly concerning neighboring peptide interaction effects on the backbone conformational distribution of short peptides and unfolded proteins. Various spectroscopic studies of a complete library of 400 dipeptides reveal that both polyproline II and beta-strand conformers are preponderant, indicating the importance of backbone peptide solvation and electronic effects. Furthermore, the thermodynamic properties determining dipeptide conformations are found to be similar to those of protein folding-unfolding processes. We anticipate that the present dipeptide library with spectroscopic data can serve as a useful database for further refinements of molecular mechanical parameters and for understanding the nature of unfolded protein structures.

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## **Theoretical studies of the protonation or deuteration reaction on aromatic compounds containing hydroxyl functional groups**

장성우, 박찬량

국민대 화학과

The mechanism of proton exchange reaction for hydroxyl-containing aromatic compounds has not been thoroughly understood although some experimental groups proposed an electrophilic substitution and tautomerization mechanism. We studied the protonation reaction of aromatic compounds containing hydroxyl groups using DFT and ab initio methods. The proton affinities were calculated using B3LYP/6-31+G(d,p) with zero-point energy corrections. The potential energy surfaces corresponding to electrophilic attack at different positions of the aromatic compounds were calculated using intrinsic reaction coordinate (IRC) method with B3LYP/6-31+G(d,p) level. Additionally the intermediates or transition states of water clusters or water mediated protonation compounds were obtained at various aromatic compounds such as phenol, catechol, resorcinol and methylcatechols to understand the proton exchange mechanism of electrophilic aromatic substitution reactions in water.

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## The optical and field emission properties of ZnO nanorods grown on p-type porous Si

이종택, 이휘건

한양대 화학과

Zinc oxide (ZnO) nanorods have shown very unique properties for applications such as field emission (FE), light emitting diode (LED), transparent film of solar cell. In general, as-synthesized ZnO nanorods have n-type semiconducting properties. In our experiment, chemical bath deposition (CBD) is used synthesis of ZnO nanorods, and precursor ZnO layer is produced by magnetron sputtering on p-type porous silicon (p-PS) for a p-n junction. Highly oriented nanorod arrays of ZnO were grown on the surface of the precursor ZnO layer by solution growth process using zinc nitrate and hexamethylenetetramine in equimolar aqueous solution. X-ray diffraction (XRD) analysis shows that the ZnO nanorods deposited on p-PS surface are non-crystalline because of the roughness of the PS surface. The photoluminescence (PL) and electroluminescence (EL) spectra from the ZnO nanorods on p-PS were obtained, which consists of blue and green emissions from ZnO nanorods and red emission from p-PS. The emission properties of ZnO nanorods on p-PS were examined due to their nanorod geometry and high aspect ratio. And the electron field emission properties of the ZnO nanorod arrays can be investigated using the Fowler–Nordheim model. It is found that the sharp geometry can substantially enhance the emission. In addition, our sample exhibits a high emission current density and a low turn-on voltage, which make it a potential candidate for further applications.

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## Separation of Metallic and Semiconducting Single-Walled Carbon Nanotubes by texturized Si substrates.

장미라, 이휘건

한양대 화학과

A single-walled nanotube (SWNT) is formed by rolling a sheet of graphene into a cylinder along an  $(m,n)$  lattice vector in the graphene plane. The  $(m,n)$  indices determine the diameter and chirality, which are key parameters of a nanotube. Depending on the chirality, SWNTs can be either metals or semiconductors, with band gaps that are relatively large or small. SWNTs have excellent mechanical and electrical properties that have led to the proposal of many potential applications. However, SWNTs are typically grown as the bundles of metallic and semiconducting tubes, thus hindering widespread applications. Therefore, it is extremely important to separate metallic and semiconducting SWNTs. Although several methods have been reported for the separation, only low yields have been achieved at great expense. we show a separation method involving different substrates process in etching solution, which makes separated SWNTs in a simple way. we compared metallic and semiconducting SWNTs by Raman spectroscopy. Raman spectroscopy is a powerful tool for the characterization of SWNTs, from which their diameter and electronic properties can be estimated.



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## The vibrational relaxation dynamics of CN stretch of $\text{SCN}^-$

김희재, 조민행

고려대 화학과

The vibrational relaxation dynamics of  $\text{SCN}^-$  anions and isotopes of  $\text{SCN}^-$  in aqueous solutions were studied by using polarization-selective IR pump-probe experiments, and the CN stretch mode frequency fluctuation and dynamics were theoretically investigated by carrying out molecular dynamics simulations of same systems. The ensemble-average-calculated linear response function associated with the IR absorption is found to be oscillating, which is in turn related to the CN stretch band shape. Numerically calculated infrared absorption spectra are directly compared with experiment and the agreement was found to be excellent. The  $T_1$  relaxation times of the CN stretch in these anions were measured by IR pump-probe spectroscopy, in which the 0-1 transition was excited, and the 1-2 transitions were monitored to follow the recovery of the ground state and decay of the excited state. For various concentration systems, relaxation rates are similar. The orientational relaxation of the CN stretch slows as the  $\text{SCN}^-$  concentration increase.

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## Static and dynamical properties of C<sub>60</sub> in organic solvents: a molecular dynamics simulation study

이지혜, 황현석

강원대 화학과

Molecular dynamics (MD) simulations are performed to study static and dynamic properties of C<sub>60</sub> molecules in typical organic molecules such as water, acetonitrile, ethanol, benzene. Radial distribution functions (RDFs) are obtained to understand the interaction between C<sub>60</sub> molecules and the organic solvents in an atomistic level. Diffusion coefficients of C<sub>60</sub> molecules in the organic solvents are also calculated and compared with experimental results. Potential of mean force (PMF) calculations as a function of the distance between two C<sub>60</sub> molecules are carried out using the umbrella sampling method with MD simulations. The PMF calculations indicate that C<sub>60</sub> molecules tend to aggregate in those organic solvents except for benzene, which is supported by the measurement of the solubility of C<sub>60</sub> in organic solvents.

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## **A molecular dynamics simulation study of structure and functions of cyclic peptide nanotubes**

서용일, 최규민, 황현석

강원대 화학과

Molecular dynamics (MD) simulations are a tool to study complex biological systems at an atomistic level. Although the method depends on the computational power, it has proven useful in investigating the structure and functions of biological molecules. In this poster, we present a MD simulation study of several types of cyclic peptide nanotubes. Potential of mean force (PMF) calculations along with MD simulations are conducted to see how the transport of ions and small biomolecules depends on the structure of cyclic peptide nanotubes. The effect of biological membranes on the transport of ions and small molecules through the cyclic peptide nanotubes are also addressed on a basis of PMF calculations.

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## Chiroptical nature of two-exciton states of light-harvesting complex : Doubly resonant three-wave-mixing spectroscopy

이호찬, \*조민행

고려대 기초과학연구소 \*고려대 화학과

Photosynthetic light-harvesting complex is a coupled multichromophore system. Due to electronic couplings between neighboring chlorophylls in the complex, the one- and two-exciton states are delocalized and they can be written as linear combinations of singly and doubly excited configurations, respectively. Despite that the chiroptical properties of one-exciton states in such a multichromophore system have been investigated by using linear optical activity measurement techniques; those of two-exciton states have not been studied before due to a lack of appropriate measurement methods. Here, we present a theoretical description on chiroptical  $\chi(2)$  spectroscopy and show that it can be used to investigate such properties of a photosynthetic light-harvesting system, which is the Fenna–Matthews–Olson complex, consisting of seven bacteriochlorophylls in its protein subunit. To simulate the doubly resonant sum- and difference-frequency-generation spectra of the complex, one- and two-exciton transition dipoles were calculated. Carrying out quantum chemistry calculations of electronically excited states of a model bacteriochlorophyll system and taking into account the dipole-induced dipole electronic transition processes between the ground state and two-exciton states, we could calculate the two-dimensional sum-frequency-generation spectra revealing dominant second-order chiroptical transition pathways and involved one- and two-exciton states. It is believed that the present computational scheme and the theoretically proposed doubly resonant two-dimensional three-wave-mixing spectroscopy would be of use to shed light on the chiroptical natures of two-exciton states of arbitrary coupled multichromophore systems.

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## The Organic Thin Film Studied by IR-ANSOM

김덕수, \*권혁상, \*김지환

고려대 기초과학연구소 \*고려대 화학과

We have investigated an infrared apertureless near-field scanning optical microscopy (IR-ANSOM) in the 3~4  $\mu\text{m}$ . As a light source, a tunable wavelength change continuous wave infrared optical parametric oscillator (cw-IR OPO) with an output power of up to 20 mW in the 3 ~ 4  $\mu\text{m}$  range has been set up. The organic thin film was prepared by deposition of octadecanethiol (ODT) self-assembled monolayer (SAM) on Au islands (thickness 40 nm) on Si substrate. We carried out sensitively organic thin film chemical mapping (C-H stretching region) of near-field around Au island nanostructures using IR-ANSOM. Clearly, the chemical map distinguishes the different components Au islands with containing ODT-SAM and Si substrate. We attained a high resolution chemical map of ODT-SAM below the diffraction limit of classical microscopy.

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## Fast non-differential Optical Rotatory Dispersion (ORD) spectrometer

엄인태, 안성현, 이한주

한국기초과학지원연구원 분석연구부

Optical rotation occurs because of difference in refractive index between left and right circularly polarized light in by optically active substance, and it is result of circular birefringence. Like circular dichroism (CD), optical rotatory dispersion (ORD) spectroscopy is very sensitive probe to molecular structure in condensed phase. We developed fast and non-differential optical rotatory dispersion (ORD) spectrometer in visible (electronic) range. Unlike conventional techniques, we used fixed linear polarization and single pulse acquisition. Especially, white light continuum generated by femtosecond laser pulse and synchronized fast CCD detector were employed, so that electronic ORD spectrum could be recorded even with single femtosecond pulse. As a result, both high signal to noise ratio and very rapid acquisition time could be simultaneously achieved.

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## Lasing properties of ZnO single nanowires

한노수, 심형섭, 서주희, 박승민, \*최명룡, 송재규

경희대 화학과 \*경상대 화학과

ZnO is a well-known wide band-gap semiconductor suitable for blue optoelectronic applications. In particular, the lasing in ZnO nanowires due to photonic confinement effects has been widely studied. With the excitation of femtosecond laser pulses, the lasing action of ZnO nanowires prepared by chemical vaporization deposition methods was observed, because the excitation pulses were shorter than the duration time of lasing. The exotic lasing in nanowires was found as a function of the excitation intensity, where the peak wavelength of lasing was blue-shifted and another peak of the longitudinal modes appeared with the increase in the excitation intensity. The mechanism of the blue-shifted lasing and the appearance of the longitudinal modes were carefully investigated. Understanding the origin of lasing modes, we have studied the polarization of the emitted light in the near UV region using polarizer and found two different polarization characters.

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## Optical properties and lasing of ZnO nanoparticles synthesized continuously in supercritical fluids

심형섭, 한노수, 서주희, 박승민, \*민병권, 송재규

경희대 화학과 \*KIST 청정에너지연구센터

Optical properties of zinc oxide (ZnO) nanoparticles prepared in supercritical methanol and supercritical water were investigated. Interstitial zinc and oxygen vacancy were the major defects in the ZnO nanoparticles synthesized in supercritical methanol. The addition of oleic acid as a surface modifier resulted in the isolation of the nanoparticles and the removal of interstitial zinc. Lasing was observed with sharp longitudinal modes and a superlinear increase in the emission intensity of the ZnO nanowires synthesized in supercritical water. The band gap renormalization due to the electron-hole plasma induced a red-shift in the emission band, whereas the individual longitudinal modes were blue-shifted due to a change in refractive index.



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## Triplet state and phosphorescence properties of PHOLED materials

서주희, 한노수, 심형섭, 박승민, 송재규

경희대 화학과

Highly efficient phosphorescent materials such as iridium and platinum complexes have attracted considerable attention for a phosphorescent organic light-emitting diode (PHOLED) with high electroluminescence efficiency because these materials can take advantage of both the electrically generated singlet and triplet excitons. High quantum efficiencies in PHOLEDs strongly depend on the energy transfer from conductive materials to luminescent ones. In other words, energy transfer from the host singlet and triplet states to the guest triplet states should be highly effective without the loss of energy for better quantum efficiencies. In addition, the energy difference between the triplet states of the host and guest molecules in the emitting layers is important for confinement of the triplet energy on the guest molecules. Luminescent properties of three types of films were investigated by temperature- and time-dependent spectroscopy. One is 4,4',4''-tris(3-methylphenylphenylamino) triphenylamine (*m*-MTDATA) films as host materials, another is *fac*-tris(2-phenyl pyridine)iridium (*fac*-Ir(ppy)<sub>3</sub>) films as highly efficient phosphorescent materials, and the third is *fac*-Ir(ppy)<sub>3</sub> doped *m*-MTDATA films.

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## Molecular Layer Deposition of Organic-Inorganic Nanohybrid Superlattice Thin Films for P-N Junction Diodes

조보람, 백장미, 성명모

한양대 화학과

We fabricated new type of organic-inorganic nano hybrid superlattice thin films by a sequential, self-limiting surface chemistry process known as molecular layer deposition (MLD) combined with atomic layer deposition (ALD). Using UV-Vis spectroscopy, we confirmed visible light absorption by LMCT. FTIR spectroscopy and XPS were employed to determine the chemical composition. Ellipsometry and TEM analysis were also used to confirm linear growth of the film versus number of MLD cycles at all same temperature. In addition, p-n junction diodes demonstrated in this study suggest that the film can be suitable for n-type semiconductors.

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## $C_{20}-X_2$ 이성체에 대한 구조와 상대적 에너지에 대한 이론 연구 (X = H, Cl)

이철, \*서영선, \*이기학

원광대 생명나노화학부 \*원광대 화학과

$C_{20}-X_2$  는 5 개의 regioisomers 를 가진다. 본 연구에서는 중성의  $C_{20}-X_2$  화합물 5 개의 regioisomers 에 대하여 구조최적화를 수행하였다 (X=H, Cl). 이들의 상대적 에너지와 각 이성체의 구조 결함 에너지를 구하여 상대적 에너지의 원인을 살펴보았다. 모든 연구는 Gaussian 03 버전을 사용하였다.

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## Single particle analysis of upconverting nanoparticles using wide-field epi-fluorescence microscope and AFM

남상환, \*배윤미, 전기석, \*\*박용일, \*\*김정현, \*최준식, 이강택, \*\*현택환, \*\*\*서영덕

한국화학연구원 나노바이오융합연구센터 \*충남대 생화학과 \*\*서울대 화학생물공학부 \*\*\*한국화학연구원 나노 바이오 융합연구센터

We carried out single particle analysis of lanthanide ion-doped upconverting nanoparticles (UCNPs) in order to compare the optical properties of various types, such as hexagonal and cubic phases, either with core or core/shell structures. UCNPs dispersed on the cover glass were imaged by both wide-field epi-fluorescence microscope and AFM. We found that the luminescence intensity of single UCNPs depended strongly on their crystal structure while there is no photoblinking for all types. We also investigated the luminescence of single PEG-phospholipid-coated UCNPs, the information from which was used to estimate the number of particles in cellular environments.

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## Real-Time Tracking of Upconverting Nanoparticles in living HeLa cells

배윤미, \*남상환, \*\*박용일, \*\*김정현, \*\*\*김형민, 최준식, \*이강택, \*\*현택환, \*\*\*\*서영덕

충남대 생화학과 \*한국화학연구원 나노바이오융합연구센터 \*\*서울대 화학생명공학부 \*\*\*한국화학연구원 융합바이오기술연구센터 \*\*\*\*한국화학연구원 나노 바이오 융합연구센터

There have been great advances in the biological imaging technology thanks to the development of nanomaterial-based probes, sensitive optical detection systems, and various analysis techniques. Here, we demonstrate the benefits of using lanthanide ion-doped upconverting nanoparticles (UCNPs) for live-cell imaging. The bright upconverted photoluminescence of UCNPs, which lies in the visible spectral range upon near-infrared (NIR) excitation, does not exhibit photoblinking and photobleaching at the single-particle level. Moreover, by employing NIR excitation, the cellular autofluorescence is totally suppressed and the degree of photodamage to cells is very low. Finally, we successfully tracked the intracellular transport of endocytosed UCNPs in real time for 6 h continuously at the frame rate of 20 frames/s.

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## **A New Technological advance for diagnosis of Parkinson Disease using PET and MRI**

조지현, \*조장근, \*안상두, 유은경, 이철현

한국기초과학지원연구원 자기공명연구부 \*중앙대 화학과

A variety of non-invasive animal imaging modalities, such as positron emission tomography (PET), computed tomography (CT), and magnetic resonance imaging (MRI), have been used as powerful tools to research human diseases. Parkinson's disease is a neurodegenerative disorder associated with aging, and patients with this disease have a deficiency of dopaminergic neurons. In the study, we evaluated fusion imaging with PET and MRI in the rat brain with [ $^{18}\text{F}$ ]FP-CIT which binds with high affinity to dopamine transporters. PET and MRI fusion images were well registered with conventional Inveon Research Workplace software, even though they are different modalities. In PET/MRI fusion images, we showed that the uptake of [ $^{18}\text{F}$ ]FP-CIT was clearly increased in the rat striatum and these images accurately matched the morphology in the rat brain atlas. PET/MRI images easily and accurately identified the regions of interest in the target tissue compared to PET/computed tomography images and enabled us to calculate the uptake of the PET tracer. Therefore, the combination of PET and MRI offers a multitude of complementary functional and anatomical information. This method could be applied to study the activity of dopaminergic neurons following changes in their morphology or after pharmacological challenges to the brain.

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## **The analysis on behavior of the iDQC and iTQC MR signals at 4.7 T animal scanner**

조지현, \*조장근, \*유효연, \*안상두, 이철현

한국기초과학지원연구원 자기공명연구부 \*중앙대 화학과

Image contrast is affected by spin density, magnetic susceptibility, molecular diffusion and perfusion, and  $T_1$  and  $T_2$  relaxation times. Relaxation times are one of the most dominant contrast-determining parameters in basic magnetic resonance (MR) imaging. So, many studies have reported the development of the contrast agent which changes the  $T_1$  and/or  $T_2$  relaxation times to enhance the image contrast. In this study, we present the experimental studies to assess the feasibility of magnetic resonance microscopy with detection of intermolecular double quantum coherence (iDQC) and intermolecular triple quantum coherence (iTQC) signals in model systems at a 4.7 T small-animal MR scanner. The characteristic behaviors of iMQC MR images depending on experimental and physical parameters are investigated. These results demonstrate the feasibility of detection and application of iMQC MR images at 4.7 T.

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## **Spin-orbit time dependent density functional theory calculation with Relativistic Effective Core Potential**

박영춘, 이윤섭

KAIST 화학과

Two-component relativistic effective core potential (RECP) is one of efficient methods including relativistic effects in various molecular systems. For the averaged relativistic effective core potential (AREP), several theories have been implemented in both ground and excited state calculations. However, excited state calculations using spin-orbit relativistic effective core potential (SOREP) have been quiet limited so far. In this poster, we present several excited state calculations of small molecules using 2-component time-dependent density functional theory (TDDFT) using SOREP. We also compare with the other several excited state methods using SOREP such as complete open shell configuration interaction (COSCI), and Fock-space coupled cluster (FSCC). All of these methods were implemented in development version of DIRAC program. For the further applications, possibilities of excited state dynamics in a few systems will also be discussed.



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## **Fluorescence spectroscopy approach to investigate the effect of pH-induced enzyme regulation by Clostridium in continuous culture**

이길용, 안태규

성균관대 에너지과학과

The biological physiology of bacteria is associated with hydronium ion concentration. Particularly Clostridium is an anaerobic bacterium that is known for its solvent-producing capabilities. The metabolism of Clostridium is characterized by the so-called acetone-butanol-ethanol (ABE) fermentation which is related to pH because ABE fermentation include acids which are acetate, butyrate and other acidic chemical. Therefore Clostridium in continuous culture changes quantities of acids which effect pH and other chemical properties include intrinsic fluorophores(autofluorescence).In this work, we investigate effect of acids and associated enzyme about intrinsic fluorophores by Fluorescence time-resolved spectroscopyE-mail address: kilyong3@gmail.com

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발표종류: 포스터, 발표일시: 금 10:30~12:30

## **Theoretical Investigation of Electronic and Structural Effects on Redox Potential of M-L Complexes Containing Nitrogen-based Ligands**

김형준, 이윤섭

KAIST 화학과

Redox flow battery(RFB) is a type of rechargeable fuel battery which produces electricity via a redox process of active materials at each electrode. Considering electronic and structural effects of nitrogen-based metal organic complexes through quantum chemical calculations, we try to suggest the active materials for RFB with high open circuit voltage above 2.5V in an effort to increase the capacity of RFB. Qualitatively, the redox potential increases for the unstable chelation with the s-character of the lone pair electrons of the N-donor atoms, the electron withdrawing ligand substituents, and especially the electron withdrawing or/and the bulky substituents directly attached to the N-donor atoms. The redox potential decreases for the stable chelation with the p-character of the lone pair electrons of the N-donor atoms, the electron donating ligand substituents, and especially the electron-rich anionic ligands. For the metal center atom, iron(III/II) redox pair is mainly analyzed.

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발표종류: 포스터, 발표일시: 금 10:30~12:30

## Ultrafast 2D-IR Vibrational Echo Spectroscopy: Acid-Base Reaction Dynamics

이주용, 조민행

고려대 화학과

Ultrafast two-dimensional infrared spectroscopy (2D-IR) is powerful as a result of simultaneously having sensitivity to molecular structure and femtosecond time-resolution for studying dynamics, which has led to successful applications in areas as varied as hydrogen bond exchange in water, chemical reaction kinetic, and peptide and protein structure and dynamics. Here, we present acid-base reaction dynamics of  $\text{CN}^-$  ion in water.

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## **Fabrication of Si-encapsulated nanoprobe for SERS imaging of multiple protein markers expressed in live cells**

이상엽, \*전향아, \*이지영, \*주재범

한양대 응용화학과 \*한양대 바이오테크놀로지학과

Raman spectroscopy is a newly developed, noninvasive preclinical imaging technique that offers picomolar sensitivity and multiplexing capabilities to the field of molecular imaging. In this study, we demonstrate the ability of Raman spectroscopy to separate the three different types of cell surface proteins in a cancer cells. Multiplexed SERS imaging of proteins on the surface of cancer cells has been carried out using functionalized core-shell nanoprobe. All types of SERS nanoprobe were successfully identified and spectrally separated using Raman imaging system. These results show great potential for multiplexed imaging in living subjects in cases in which several targeted SERS probes could offer better detection of multiple biomarkers associated with a specific disease.

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발표종류: 포스터, 발표일시: 금 10:30~12:30

## **A new sampling and scoring method for high-resolution protein-protein docking**

이하섭, 박한범, 석차욱

서울대 화학부

Protein-protein interactions play key roles in many cellular pathways. Computational docking study of protein-protein complexes enables us to explore quaternary structures of interest even when experimental data are not available. In particular, prediction of quaternary structures in high-resolution is crucial to obtain valuable insights into protein-protein interactions in molecular details. An initial stage docking tool, ZDOCK, is widely used to obtain rough docking poses. It employs a coarse-grained score function that considers shape complementarity, desolvation, and electrostatics. In this study, we developed a new sampling method and a score function for prediction of high-resolution protein-protein complex structures starting from the initial stage docking results. The sampling method utilizes an extensive search algorithm that can efficiently search important degrees of freedom of a given system. The score function is based on physicochemical properties and statistical preferences of amino acids and is represented by a weighted sum of van der Waals, electrostatic, desolvation, conservation, statistical, and hydrogen bonding energies. The performance of the new method is tested on the ZDOCK benchmark set.

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## **Consistent Production of the Protective Layered Hollow Gold Nanospheres (Silica/Polymer/Au) for the Multiplex Surface-Enhanced Raman Scattering Detection**

김기형, \*주재범

한양대 바이오 나노공학과 \*한양대 생명나노공학과

The use of silica shells offers many advantages for the surface-enhanced Raman scattering (SERS)-based biosensing applications in terms of its optical transparency, remarkable stability and improved biocompatibility. In this presentation, we report a novel polymer-assisted preparation method to obtain the silica-coated hollow gold nanosphere (HGN) SERS tags. Poly(acrylic acid) was used to stabilize the dye-tagged HGNs before adsorbing the coupling agent and then silica shell was deposited onto the particle surface by the Stöber's method. The unwanted competitive adsorption between Raman reporter molecules and coupling agents, which results in inconsistent loading of reporter molecules on the individual nanoparticles, could be avoided by this method. The proposed silica-coated HGN tags showed strong SERS signals as well as excellent multiplexing capabilities.

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## Application of Silver-Coated Magnetic Microspheres to a SERS-Based Optofluidic Sensor

정은수, 최남현, 박세휘, 이남우, 르레호만, \*주재범

한양대 바이오나노공학과 \*한양대 생명나노공학과

Silver-coated magnetic microspheres ( $\text{Fe}_3\text{O}_4/\text{Ag}$  core/shell) were fabricated to use them as a surface-enhanced Raman scattering (SERS) substrate. Magnetic microspheres are prepared through two steps. First, gold (AuNPs) were seeded by electrostatic force on the surface of microspheres. Then, Au seeded microspheres are reduced by Ag ions and they were grown up again. These magnetic microspheres have been characterized using Raman spectroscopy, field emission scanning electron microscopy (FE-SEM), field emission transmission electron microscopy (FE-TEM) and energy dispersive Spectroscopy (EDS). For trace analysis in a microfluidic channel, a microfluidic device integrated with solenoids has been fabricated. The solenoid chip allowed us to control the alignment of the magnetic microspheres on the wall of the microfluidic channel. Target samples were introduced into the channel and adsorbed on the surface of trapped silver-coated magnetic microspheres. SERS signals were then measured using a confocal Raman microscope. It is believed that a SERS-based optofluidic sensor with silver-coated magnetic microspheres can be successfully applied to micro-environmental analysis and other highly sensitive bio-analyses.

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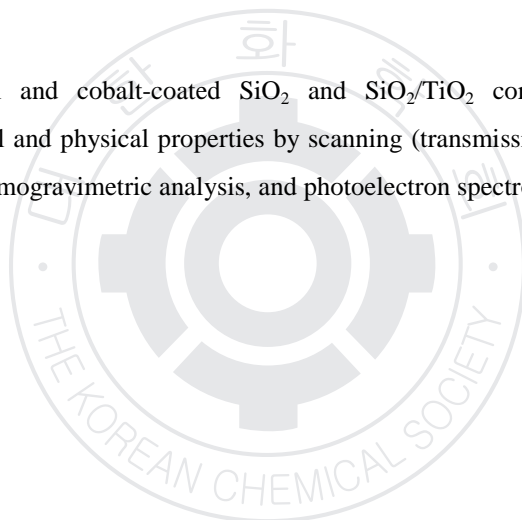
발표종류: 포스터, 발표일시: 금 10:30~12:30

## Ni- and Co-coated SiO<sub>2</sub> and SiO<sub>2</sub>/TiO<sub>2</sub> core-shell nanostructures

손영구, 도예지

영남대 화학과

We have prepared nickel and cobalt-coated SiO<sub>2</sub> and SiO<sub>2</sub>/TiO<sub>2</sub> core-shell nanostructures, and characterized their chemical and physical properties by scanning (transmission) electron microscopy, X-ray diffraction method, thermogravimetric analysis, and photoelectron spectroscopy.





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발표종류: 포스터, 발표일시: 금 10:30~12:30

## Relativistic effect modified compound methods: benchmark for group 13 element hydride dimers

박지영, 박영춘, 이윤섭

KAIST 화학과

For obtaining the accurate thermo-chemical data while low computational cost is maintained, various compound methods are developed. One of the most famous methods, Gaussian-n set covers most of organic molecules. But relativistic effect correction is not enough on this Gaussian-n set because relativistic effect correction is not strongly required for light elements. Unlike these molecules including light elements, relativistic effect should be mainly considered for describing the molecules including heavy element, Relativistic effect modified compound methods is consisted by optimization step, single point correction step, and higher-level correction step. First, we tested some DFT functions for geometric properties. From the most proper DFT calculated structure, single point correction of polarization, diffuse function, and correlation effect is obtained. Finally, spin-orbit correction is included. For each step, relativistic effect included calculation was compared with not included one. Some test calculations were performed with hydride dimers of group 13 elements,  $(\text{GaH})_2$ ,  $(\text{InH})_2$ , and  $(\text{TlH})_2$ .

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## **siRNA delivery using NH<sub>2</sub>-PEG-modified gold nanoparticles directed into gastric cancer cells.**

정새로미, 주상우

승실대 화학과

Development of the effective delivery of RNA therapeutics agents has gained increasing attention for various disease treatments by suppressing specific genes. Due to inefficient transfection of RNA therapeutics, novel drug delivery systems are currently in need. Gold nanoparticle (Au NP) delivery system wrapped with the polycations of branched - polyethylenimine (BPEI) was used to fabricate a complex conjugate of siRNA-BPEI AuNPs for a small interference RNA (siRNA) delivery system. The synthesis of the siRNA-BPEI Au NPs conjugates was conducted by modifying Au NPs with HS-PEG-NH<sub>2</sub>. After 3-(2-pyridyldithio)-propionic acid N-hydroxysuccinimide ester (SPDP) was linked to HS-PEG-Au NPs, we conjugated thiolated siRNA to SPDP by the addition of excessive HS-siRNA. UV-Vis and infrared spectroscopy was used to check the assemblies of siRNA on Au NPs. The genes related to voltage-gated K<sup>+</sup> channel proteins in gastric cancer cells were targeted to design a siRNA sequence. Gene silencing effects were examined by PCR methods. We plan to check the internalization of siRNA-loaded Au NPs by Raman spectroscopy and transmission electron microscopy. Our results may suggest that our siRNA delivery system (SPDP-PEG-BPEI Au NPs) should be potentially suitable for RNAi therapy.

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발표종류: 포스터, 발표일시: 금 10:30~12:30

## **Folate receptor targeted drug delivery systems using gold nanoparticles directed into cancer cells**

박진, 주상우

승실대 화학과

Since the folic acid receptors are frequently over-expressed on the surfaces of human cancer cells, folic acid can be a useful the conjugation of folic acid on gold nanoparticle (AuNPs) surfaces embedded with anticancer drugs is studied by spectroscopic tools. Purine analogues such as 6-Mercaptopurine and thioguanine are used as anticancer drugs. Folic acid is conjugated to AuNPs surface modified with 4-aminothiophenol via an 1-ethyl-3-[3-dimethylaminopropyl]carbodiimide hydrochloride (EDC) reaction coupling. Transmission electron microscopy, dark field microscopy, and surface enhanced Raman scattering were used to monitor the cellular uptake of folate-receptor targeted AuNPs. Folate receptor-positive HeLa and folate receptor-negative A549 cells were compared to check the internalization of AuNPs. Cell viability test using a CCK-8 assay indicated that folate receptor targeted AuNPs exhibited an enhanced efficacy of anticancer drug activities.

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발표종류: 포스터, 발표일시: 금 10:30~12:30

## Conjugation of Anticancer Drugs on Nanoparticles Characterized by Spectroscopic Tools

Ganbold Erdene Ochir, 주상우

승실대 화학과

Recently, nanoparticle (NP)-based cancer therapy has received much attention in nanotherapeutics. We are studying the bio-conjugated systems of anticancer drug molecules on noble metal and semiconductor NP surfaces by self-assembly. Gold NPs have gained great interest in the safe and efficient drug delivery systems due to their low toxicity and biocompatibility. Since purine or pyrimidine analogue drugs attached to Au NP surface were found to exhibit fairly strong Raman signal, the z-depth Raman measurement could be a useful tool to observe information on the localization of Au NP-drug conjugates. Confocal Raman spectroscopy and dark-field microscopy are performed to monitor the localization of the drug-embedded AuNPs inside the cell. UV-Visible and Raman spectra have shown that drug molecules are adsorbed on Au NP surfaces via chemical bonds. Several cancer cells are used to check the enhanced efficacy for these drug-conjugated NPs by measuring the cell viability. In this presentation, we introduced several anticancer drug molecule-Au NP conjugate systems toward their improved efficacies.

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발표종류: 포스터, 발표일시: 금 10:30~12:30

## **Paclitaxel conjugated to ZnO and TiO<sub>2</sub> nanoparticles directed into cancer cell**

서지혜, 주상우

승실대 화학과

Paclitaxel is one of the most widely used anticancer chemotherapy agents to treat various cancers. In this work, we study the conjugation of paclitaxel on ZnO, TiO<sub>2</sub>, and Ag/AgBr/TiO<sub>2</sub> nanoparticles. Infrared spectroscopy was used to examine the adsorption of paclitaxel. Fluorescence microscopy was used to check the cellular uptake as well as the disruption of microtubules inside the cancer cells. We plan to compare the cell viability of paclitaxel-nanoparticle conjugates before and after assembly by MTT or CCK-8 analysis. Light-induced cancer cell killing effects will also be examined to induce the photocatalytic effects in addition. Our drug-nanoparticle conjugate systems are expected to be potentially useful for cancer nanotherapeutics.

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발표종류: 포스터, 발표일시: 금 10:30~12:30

## **Infrared spectroscopy of ZnO functionalization for protein conjugation**

우린토야, 주상우

승실대 화학과

Nanoparticles (NP) exhibit novel physicochemical properties that can be applied to biological substrates and processes. Recently ZnO NPs have been used in wide areas of biosensor, biomaterial, cell imaging, and material sciences. In this work, we assembled 16-phosphohexadecanoic acid to link proteins on ZnO NP surfaces. We conjugated the amino groups of bovine serum albumin and transferrin proteins to the surface carboxyl groups on 16-phosphohexadecanoic acid-assembled ZnO nanoparticle via an (1-ethyl-3-[3-dimethylaminopropyl] carbodiimide hydrochloride) (EDC)-coupling. The structures of ZnO NPs are examined by UV-vis and X-ray diffraction spectroscopic tools. We characterize the functionalization of ZnO NPs by Fourier-Transform infrared spectroscopy. We plan to conjugate some monoclonal antibodies for the targeted drug delivery and also use TEM-EDAX or ICP-MS and DLS (dynamic light scattering, zeta potential measurements) to monitor the cellular uptake of ZnO NPs.

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## **In vitro glutathione-triggered drug release inside a single cell by label-free Raman spectroscopy**

옥광수, 주상우

승실대 화학과

Stimulated-drug release is of significance to achieve a controlled and efficacious treatment of cancer cells. Recently, nanoparticles have been widely used for more efficient drug delivery systems. Gold nanoparticles are one of the promising drug carriers, because of their bio-compatibility and easiness to control surface modification. The purpose of this research is to examine glutathione-induced drug release by Raman spectroscopy. Two purine analogue anti-cancer drugs are tested for the label-free Raman experiments. 6-Mercaptopurine and 6-thioguanine are found to adsorb on gold by either Au-S linkages or Au-N bonds. Glutathione was found to reduce the oxidized Au-S linkages and make the drug molecules released, resulting in decrease of Raman intensities. Our method is a useful way to estimate in-situ drug release inside a single cell from the gold nanoparticle-based drug delivery systems.

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발표종류: 포스터, 발표일시: 금 10:30~12:30

## Gold Nanoparticle Conjugates of Gefinitib and Erlotinib Directed into Lung Cancer Cells

김세미, 주상우

승실대 화학과

Inhibitors of epidermal growth factor receptor or tyrosine kinase are currently used on the market to cure various cancer-related diseases. Gefinitib (GF) and erlotinib (EL) are the two most popular and commercially available drugs to treat non-small-cell lung cancers. Gold nanoparticles (AuNPs) have been introduced as novel drug delivery systems to enhance the efficacies of drugs. We fabricated the AuNP conjugates of GF and EL to test their potency toward lung cancer cells of A549 and NCI H460. The adsorption of GF and EL on AuNP surfaces were examined by UV-Vis and surface-enhanced Raman scattering. GF and EL appeared to adsorb on Au NP surfaces via the N-Au bond and the acetylide-Au linkage, respectively. The internalizations of AuNPs are examined by transmission electron microscopy and confocal Raman spectroscopy. Cell viability tests of free GF and EL in comparison with their AuNP conjugates into A549 and NCI H460 cells are currently in progress by CCK-8 analysis. We hope that our method can be utilized as a potentially useful drug delivery system to enhance the efficacies for treating lung cancer cells.



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발표종류: 포스터, 발표일시: 금 10:30~12:30

## Adsorption of self-assembled monolayers on ZnO nanoparticles

김미라, 주상우

승실대 화학과

We study the adsorption of self-assembled monolayers on ZnO nanoparticles using vibrational spectroscopy tools. 4-Mercatopurine and 4-mercaptobenzoic acid on ZnO nanoparticle surfaces were examined by means of wavelength-dependent Raman spectroscopy. The irradiations of excitation wavelengths at 325, 532, 633, 785 and 1064 nm are currently under examination to investigate the wavelength dependent Raman spectral behaviors of the self-assembled monolayers on ZnO nanoparticles. Charge-transfer mechanisms appeared to play a role in the enhancement of Raman intensities. UV-Vis spectra were obtained to explain the electronic absorption bands. We plan to assemble other drug molecules on ZnO nanoparticle surfaces to aim at a potential usage in the drug delivery systems.

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발표코드: III-PHYS.P-202

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발표종류: 포스터, 발표일시: 금 10:30~12:30

## Structure and optical properties of ZnO synthesized by sol-gel method

박병천, 김재욱, 차병관, 김종규

단국대 화학과

ZnO- synthesized by sol-gel method was investigated. Components of chemical compound were checked by X-ray diffraction (XRD). When the value of NaOH and KOH was added into ZnO, 101 peak of ZnO was altered to shape. Morphology of ZnO was captured by Scanning electron microscope (SEM). Variation of morphology of ZnO was changed from cuboid to rod. To find optical property of ZnO, the sample solution which mixed both ZnO and dye(methylene blue) was radiated using UV-lamp (254nm). And it was checked operating UV-Vis spectroscopy. Absorbance of ZnO was decreased as adding the each of the ZnO. and peak of absorbance of ZnO was depended by the time of irradiation at the sample solution.

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발표코드: III-PHYS.P-203

발표분야: 물리화학

발표종류: 포스터, 발표일시: 금 10:30~12:30

## **The constitution of nanostructures of Cu<sub>2</sub>O synthesized by a simple way of hydrothermal method.**

차병관, 김재욱, 김종규

단국대 화학과

Nanostructures of Cu<sub>2</sub>O powders were synthesised via hydrothermal technique. The products were prepared using Copper acetate mono-hydrate, Lactic acid and various alcohols. Lactic acid with distilled water was used as the acidic catalyst to control the hydrolysis reaction, and the morphology of Cu<sub>2</sub>O powders was changed due to various alcohols. In this current study, the effects of reaction on the product morphology as well as crystallization mechanism were examined by using X-ray diffraction (XRD), scanning electron microscopy (SEM). It was found that morphology of Cu<sub>2</sub>O powders was changed in various alcohols.

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발표종류: 포스터, 발표일시: 금 10:30~12:30

## Theoretical and experimental study of the Glycolic acid in a Ar matrix

이슬기, 최명룡

경상대 화학과

The glycolic acid in argon has been investigated by low temperature matrix isolation spectroscopy. We have coupled a home built supersonic jet system with matrix isolation FT-IR spectrometry to study the conformation of glycolic acid at low temperature(10K). We are deposited to the matrix were measured by FT-IR spectroscopy. For the interpretation of the obtained experimental data the results of ab initio calculation was DFT level of theory using the Gaussian 03 program with B3LYP/6-311(d,p) basis set.

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발표코드: IV-ANAL.P-1

발표분야: 분석화학

발표종류: 포스터, 발표일시: 금 15:00~17:00

## Quantification of Self-Exchange of Alkanethiol with Deuterated Alkanethiol on SAMs Using MALDI-TOF MS

강현욱, 여운석

건국대 생명공학과

Self-assembled monolayers (SAMs) of alkanethiolates on gold are key elements for chemical/biochemical applications such as biosensors, biochips, actuators, and molecular electronics. Many of the factors such as immersion time, temperature, solvent, and a carbon number of alkyl chain affect the SAM growth process, adsorption and desorption, and self-exchange of alkanethiols. However, effective methods for the quantitative analysis of these affects are not present. In this poster, we describe the analysis of the self-exchange of alkanethiols on gold surface using matrix assisted laser desorption/ionization time of flight (MALDI-TOF) MS. The composition and chemical/biochemical conversion of alkanethiolates of SAMs can be analyzed by MALDI-TOF MS simply, rapidly and directly. For this study, we used the deuterated alkanethiol that has same molecular properties but different molecular weight as non-deuterated alkanethiol. SAMs on gold consisting of non-deuterated alkanethiol was immersed into deuterated alkanethiol solution to determine the rate of self-exchange with different immersion time, solvent, and length of alkanethiol. The self-exchange rate at difference conditions was directly analyzed by MALDI-TOF-MS, which gave the pseudo-first-order kinetics. We believe our research will be used as characterization method for practical application such as existing chemical patterning techniques, dynamic monolayer gradients, and fabrication of monolayer films by affording high precision and quantitative information.

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발표코드: IV-ANAL.P-2

발표분야: 분석화학

발표종류: 포스터, 발표일시: 금 15:00~17:00

## Quantification of Proteins on Several Types of Nanoparticles

주수미, 여운석

건국대 생명공학과

Protein coated nanomaterials have become useful research tools of great significance due to its versatility in biomedical and biosensor applications. In particular, protein-coated nanoparticles (NPs) have been used in many studies such as drug delivery, disease diagnosis, therapeutics, and bioassay. Amount and density of proteins on a particles' surface are important parameters that need to be calculable in most applications. While quantification methods for two dimensional surface-bound proteins are common such as surface plasmon resonance (SPR), quartz crystal microbalance measurements (QCM), and enzyme-linked immunosorbent assay (ELISA), the efficient method for quantification of proteins on three dimensional surfaces has not been reported yet. In this poster, we report a new protocol for the quantification of proteins on several types of NPs using matrix assisted laser desorption/ionization time of flight (MALDI-TOF) MS. The nanoparticle-bound protein was digested by trypsin and the resulting peptide fragments were analyzed by MALDI-TOF MS after addition of an isotope-labeled internal standard (IS). The IS, which has the same sequence as a representative peptide of the surface bound protein, was added in a known quantity to the digest, and thus allowed absolute quantitation of proteins on nanoparticles by comparing the mass intensities between the representative peptide and the IS. As model systems, hollow gold nanoparticles (HGN) and silica nanoparticles (SNP) were tested using bovine serum albumin (BSA) and glutathione S-transferase (GST) as coating proteins. We believe this method will be useful by providing the quantitative information for the many studies in bioapplications.

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장소: 제주ICC

발표코드: IV-ANAL.P-3

발표분야: 분석화학

발표종류: 포스터, 발표일시: 금 15:00~17:00

## Generation and characterization of surface gradient having kinetic property

이정욱, 여운석

건국대 생명공학과

Surface gradient (heptotaxis) is crucial in embryonic development, inflammatory immune response, wound repair, tumor formation and metastasis. Generating the gradient of biomolecules on the surface is important to study effective therapeutic approaches for treating diseases, understanding cell proliferation, and preparation of artificial tissue. Most current techniques of generating surface gradient require complex instruments, high level of operating control, and expensive cost. In addition, they are limited in their ability to maintain gradient over a long period of time. In this poster, we describe a new method for generation of the gradient on a surface using chemically reactive quinone-derivatives. Our strategy utilizes self-assembled monolayers (SAMs) on gold consisting of alkanethiolates which were terminated by chemically reactive quinone-derivatives. Upon a reduction of quinone moiety to corresponding hydroquinone by a reducing agent, cyclization reaction ensues to give the amine functionality. This cyclization reaction takes a few minutes to complete and therefore, the exposure time of the monolayer to the reducing agent is proportional to the density of amine on the surface. A kinetic model based on first-order kinetics is used to afford initial rates and half-life of the reaction. To verify our strategy, the amine gradient was conjugated with amine-specific fluorescent die and the cell adhesion ligand, RGD peptide. As expected, we obtained the fluorescence gradient and the cell population gradient in accordance with the amine gradient. We believe this strategy using chemical reaction to generate gradient would be useful in many applications for biological researches.

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장소: 제주ICC

발표코드: IV-ANAL.P-4

발표분야: 분석화학

발표종류: 포스터, 발표일시: 금 15:00~17:00

## Determination of trace elements in high purity molybdenum by Laser ablation Inductively Coupled Plasma Mass Spectrometry

정세훈, \*박종일, 고재윤, 허성우

포항공과대 화학과 \*포항산업과학연구원 원천소재 연구센터

It is very important to analyze the contents of impurity elements such as W, Nb, Cr, Fe, and so on in the high purity molybdenum. A laser ablation system is a useful technique for rapid and quantitative analysis in atomic spectrometry by direct nebulization. In this study, determination of impurity elements in high purity molybdenum was performed by inductively coupled plasma mass spectrometry with laser ablation (ICP-MS). The laser ablation system consists of a 213 nm Q-switched Nd:YAG laser and He carrier gas. The samples were directly nebulized into ICP-MS as the optimized power of intensity and stability of analytic elements with scanning mode. The analytical concentrations of the molybdenum samples using laser ablation-ICP-MS were compared with glow discharge mass spectrometry (GD-MS) and conventional solution ICP-MS with matrix separation in both accuracy and precision. The correlation coefficients between the concentrations and the intensity ratio, and the relative standard deviation have good results. Consequently, laser ablation ICP-MS could be rapid and quantitative technique to determine trace elements in molybdenum under the ng/g levels.



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장소: 제주ICC

발표코드: IV-ANAL.P-5

발표분야: 분석화학

발표종류: 포스터, 발표일시: 금 15:00~17:00

## Determination of Optimum Sensitivity for DNA Microarray

이주운

충주대 교양학부 - 화학

Mechanically spotted DNA microarray technology has become a powerful tool for the investigation of gene expression and transcription analysis in a high-throughput manner. The objective of this study is to evaluate commercially available microarray slides and chemically modified DNA probes along with variation of spotting solution in terms of array sensitivity. Four different types of microarray slides, two different functional group linkers modified for nucleic acid probe, and glycerol content in spotting solution were evaluated. Microarray slides from Nexterion<sup>®</sup> coated with epoxy show highest signal intensity regardless of linker functional group. Addition of glycerol in spotting solution also improves the signal strength in general. Although this study is limited to particular commercial slides and chemical information of linker group is not disclosed by vendors, the work successfully demonstrates that optimum arraying protocol can be achieved and any incompatibilities of certain combinations can be found and avoided for future microarray spotting.

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장소: 제주ICC

발표코드: IV-ANAL.P-6

발표분야: 분석화학

발표종류: 포스터, 발표일시: 금 15:00~17:00

## **Fast separations of chiral $\beta$ -blockers on a cellulose tris(3,5-dimethylphenylcarbamate)-coated zirconia monolithic column by capillary electrochromatography**

박진명, 김민지, 이정미, 홍종성, 박정학

영남대 화학과

Cellulose tris(3,5-dimethylphenylcarbamate) (CDMPC) is an excellent chiral selector for enantioseparation of a wide variety of chiral compounds. The monolithic chiral columns are becoming popular in liquid chromatography and capillary electrochromatography. In this work, we present the fast separation of chiral  $\beta$ -blockers on a CDMPC-modified zirconia monolithic column by capillary electrochromatography (CEC). The porous zirconia monolithic capillary column was prepared by using the sol-gel technology and then zirconia surface modified with CDMPC. The enantioseparations were performed in reversed-phase (RP) eluents of a phosphate solution (pH 4.4) modified with acetonitrile or alcohol. The enantioseparations of a set of ten chiral  $\beta$ -blockers were achieved in less than one minute. Influences of the applied voltage, column temperature, concentration of acetonitrile and the type of alcohol as the organic modifier in the mobile phase, and sample injection time on enantioseparation were investigated. CEC separations at the applied voltage of 10 kV and 15°C in the ACN-modified mobile phase provided the best resolutions for the analytes studied. Run-to-run and day-to-day repeatabilities of the column in the RP-CEC separation were less than 1 and 2 %, respectively.

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장소: 제주ICC

발표코드: IV-ANAL.P-7

발표분야: 분석화학

발표종류: 포스터, 발표일시: 금 15:00~17:00

## Identification of Phospholipids in Mouse Brain by using MALDI TOF-TOF

박영승, 김정권, \*김광표, \*\*김영환

충남대 화학과 \*건국대 분자생명공학과 \*\*한국기초과학지원연구원 질량분석연구부

Lipids with relative composition within the cell are dynamic because of numerous pathways involved in their biosynthesis and turnover. However, their mass spectral profilings were very complex and not quantitative due to the alkali metal adduction of lipid species with  $\text{Na}^+$  and  $\text{K}^+$  ions present in biological samples. Thus, the mass spectra of lipids ionized by ESI and MALDI indicate simultaneously sodiated, potassiated and protonated molecules of the same species. In this study, the sodium-adducted molecules of lipid species were exclusively observed in MALDI mass spectra by using matrix saturated with sodium acetate. We also determined the polar head group and two fatty acyl compositions of the sodium-adducted molecules of phospholipids by high-energy tandem mass spectrometry with MALDI TOF/TOF. In addition, the results of this study will be applied to MALDI imaging mass spectrometry (IMS) of phospholipids directly on brain tissue section.

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장소: 제주ICC

발표코드: IV-ANAL.P-8

발표분야: 분석화학

발표종류: 포스터, 발표일시: 금 15:00~17:00

## Association between urinary bisphenol-A concentration and estrogens

김은지, \*정봉철, \*\*이정애

고려대 생명공학과 \*KIST 생체대사연구센터 \*\*KIST 생체대사연구센터

Bisphenol-A(BPA), known as major environmental endocrine disrupting chemicals, is a monomer used to make polycarbonate, such as the lining of food and epoxy resins and have estrogenic properties both in vitro and in vivo. It may be able to enter the body by ingestion or adsorption in many way due to exposure to high temperature and acid or base condition so that incomplete polymerization. However, exposures to BPA at low levels have been interference with steroid hormone receptors such as estrogen receptor and androgen receptor and may bring about negative effect in body's own hormones. The present study was designed to analyzed urinary estrogens association with high group of BPA ( $n=100$ ,  $11.05 \pm 20.47$  ug/g creatinine) and low group of BPA ( $n=100$ ,  $0.07 \pm 0.22$  ug/g creatinine) using gas chromatography-mass spectrometry. These methods contain solid-phase extraction with Oasis HLB C18, enzymatic hydrolysis, liquid-liquid extraction using ethyl acetate:n-hexane (2:3,v/v) and following conversion to trimethylsilyl derivatives for sensitive analysis in the selected ion-monitoring mode. As a result, an estrogen level of the high group of BPA was increased in both men and women when compared to the low group of BPA. Especially, the level of 4-hydroxyestradiol(4-OH-E2) was increased to compare with 2-hydroxyestradiol in the high group of BPA, which it resulted from 4-hydroxylase and this enzyme consequently produced quinone that it might act as a carcinogen. For that reason, high level of 4-OH-E2 lead to oxidative damage to lipids, proteins and DNA as a result of production of reactive oxygen species. In conclusion, an increased level of 4-OH-E2 and an increased activity of 4-hydroxyestrogen might elevate the risk due to formation of quinone, DNA damage and therefore initiation of cancer.

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장소: 제주ICC

발표코드: IV-ANAL.P-9

발표분야: 분석화학

발표종류: 포스터, 발표일시: 금 15:00~17:00

## Carbon nanofibers grown on Co(II) deposited solid carbon foam

김태윤, 박시내, 이창섭

계명대 화학과

This study investigates carbon nanofibers grown on solid carbon foam by catalytic decomposition of ethylene. Polyurethane helps to cause aging in regins (KR-65, DH-40) after carbon foam was carbonized. After 6 hours of aging time, polyurethane resin melted and carbon skeleton was foamed. Prior to cobalt deposition, the carbon foam templates were oxidized by refluxing in concentrated nitric acid for 60 min. The oxidation creates oxygen containing surface groups on carbon foam which acts as anchoring sites on which the cobalt precursor can nucleate and anchor. A Cobalt(II) concentration of 5gCo/gRVC results in fibers with a diameter of 50 to 100 nm. The effect of cobalt loading on fiber diameter and morphology and fiber layer thickness was studied using SEM.

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장소: 제주ICC

발표코드: IV-ANAL.P-10

발표분야: 분석화학

발표종류: 포스터, 발표일시: 금 15:00~17:00

## Synthesis of carbon nanofiber supported on Iron catalysts

현유라, 이창섭, 전동환

계명대 화학과

his study focuses on the synthesis of carbon nanofibers (CNFs) on solid carbon foam. The purpose of the CNFs is to enlarge the surface area of the reticulated vitreous carbon(RVC) foam and the combination of CNFs with RVC foam can be used as a catalyst support. The CNFs in the study have been synthesized using iron catalyst and ethylene as a carbon source. The iron has been deposited on the RVC foam using homogeneous deposition precipitation. The influence of both iron content in the precursor solution and deposition time on the CNF coverage of the RVC surface, fiber thickness, and surface area has been studied. Polyacrylonitrile(PAN) and  $\text{Fe}(\text{acac})_3$  mixture was dissolved together in dimethylformamide(DMF) with a concentration of 9wt% and 3.8wt%, respectively, and put polyurethane foam into the solution. The sample were calendered after oxidation and cured at 250 °C in air for 9 hrs. Stabilization and carbonization of PAN and the reduction of the  $\text{Fe}^{3+}$  were completed in a high-temperature furnace by the following steps: 1) heating up to 600 °C at a rate of 10 °C/min a mixture of  $\text{H}_2$  and Ar for 4h to reduce the  $\text{Fe}^{3+}$  to Fe; 2) heating up to 1100 °C in Ar at a rate 5 °C/min for 30min to pyrolysis; 3) CNFs synthesis in mixture of 21% ethylene and  $\text{H}_2/\text{Ar}$  at 700 °C for 2h in CVD process. Finally structural characterization of the CNFs was performed by SEM and composition analysis was carried out using EDX.

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장소: 제주ICC

발표코드: IV-ANAL.P-11

발표분야: 분석화학

발표종류: 포스터, 발표일시: 금 15:00~17:00

## 1H/15N Solid-state NMR Probe for oriented membrane proteins

박태준, 최성섭, 김지선, 김용애

한국외국어대 화학과

X-ray crystallography and conventional solution NMR spectroscopy techniques are difficult to use for the study of membrane protein structures, because the lipids required for the structural integrity and functionality of the membrane proteins prevent the crystallization of the proteins as well as reducing their rate of overall reorientation in solution. A lipid bilayer provides the protein with a physical and chemical environment most similar to a natural membrane, but the large size and slow tumbling of lipid bilayer require the use of solid-state NMR methods. Solid-state NMR experiments on lipid bilayers or bicelle samples are valuable for membrane proteins with a predominantly helical secondary structure. The orientational restraints from membrane proteins in a lipid environment could be obtained by 1H-15N heteronuclear dipolar coupling solid-state NMR experiments, PISEMA or SAMMY. 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. Moreover, these biological samples are readily heated and destabilized during radio frequency irradiation. 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 400 MHz wide-bore 1H-15N solid-state NMR probe with 5-mm solenoidal rf coil and an 800 MHz narrow-bore 1H-15N solid-state NMR probe with strip-shield coil for high power, multi-pulse sequence experiments, such as 2D PISEMA or 2D SAMMY. These probes provide 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 were successfully obtained by using these home-built solid-state NMR probe. In addition, we will present the

ongoing constructions 400MHz wide-bore and 500 MHz narrow-bore  $^{19}\text{F}$ - $^{13}\text{C}$  solid-state NMR probe for in-situ analysis of liquid crystal display panels in display industry.





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발표코드: IV-ANAL.P-12

발표분야: 분석화학

발표종류: 포스터, 발표일시: 금 15:00~17:00

## **Development of an Analytical Method for Glycoprotein Separation based on Lectin-immobilized Beads with Flow Field-Flow Fractionation**

김진용, 문명희

연세대 화학과

Glycosylation of protein is playing a key role in critical biological processes including protein folding, cellular adhesion, immunological recognition, signaling, and disease progression. The failure of such protein glycosylation can cause a variety of diseases. Therefore glycoprotein study is clinically important but it is not simple due to low abundance of glycopeptides from typical biological samples. Lectins are particularly capable of selective binding with certain type of glycans attached to protein. Lectin affinity chromatography using such property of lectins has been utilized for isolation of glycoproteins, however there are some limitations in analysis of glycoproteins. In this study, we are developing an analytical method for identification of glycoproteins to overcome the limitations of conventional analytical methods. We immobilized different lectins on silica particles with different sizes, and then utilized different affinities of standard glycoproteins to each lectin-immobilized silica beads. Separation of these silica particles in accordance with their size was performed by using flow field-flow fractionation (FIFFF). By using the reagent creating fluorescent signal on glycoproteins, stained particles were quantitatively elucidated. Furthermore, size fractionated lectin-immobilized beads were collected during FIFFF run for further characterization of glycoproteins using the shotgun proteomic method. Initial evaluations were made with standard glycoproteins.

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장소: 제주ICC

발표코드: IV-ANAL.P-13

발표분야: 분석화학

발표종류: 포스터, 발표일시: 금 15:00~17:00

## Quantitative analysis of Phospholipids from Prostate Cancer Cell Lines treated with D-Allose Using Nano-flow LC-ESI-MS-MS

임상수, 문명희

연세대 화학과

Lipidomics is the comprehensive study of networks of cellular lipids in throughout biological systems. It is of increasing interests to study the changes in lipid compositions and their comparative abundances in various biological candidates due to its metabolic functions. Among various kinds of lipids, phospholipids (PLs) are major components of cellular membrane and composed of mixtures of various molecular species depending on their type of head groups and two acyl chains. In this study, nano-flow liquid chromatography combined with electrospray ionization tandem mass spectrometry (LC-ESI-MS-MS) was utilized for the identification and comparison of PLs in prostate cancer cell lines (PrEC, DU145, LNCaP) with and without D-allose treatment. D-allose is a monosaccharide present in minute quantities in nature and a rare sugar used as an anti-cancer drug (breast cancer or, prostate cancer) without any side effects. Separation of phospholipids are carried out using a homemade reversed phase capillary column with binary solvents and the mass spectrometry experiment of eluted PLs was performed at the precursor scan first and followed by data dependent MS/MS scan events. Quantitative analysis of PC (phosphatidylcholine), PE (phosphatidylethanolamine), PS (phosphatidylserine), PI (phosphatidylinositol), PG (phosphatidylglycerol) and PA (phosphatidic acid) for the cell lines with and without the treatment of D-allose are carried out, and the PLs of which have a significant difference in their distributions are chosen and statistically investigated through principal component analysis(PCA) for the discovery of potential biomarkers of prostate cancer.

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장소: 제주ICC

발표코드: IV-ANAL.P-14

발표분야: 분석화학

발표종류: 포스터, 발표일시: 금 15:00~17:00

## Characterization of Plasma Lipoprotein Phospholipids from Patients with Coronary Artery Disease by Flow Field-Flow Fractionation and Nanoflow LC-ESI-MS-MS

변슬기, \*이주용, \*문명희

연세대 화학 \*연세대 화학과

High-density lipoproteins (HDL) and low-density lipoproteins (LDL) are purported to have a correlational relationship with a potential risk of developing various heart diseases and among them, coronary artery disease (CAD) has emerged as one of the common ones throughout the world. Low levels of high-density lipoprotein and high levels of low-density lipoprotein contribute to pathogenesis of CAD and many studies have been mainly focused on quantitative analysis of lipoproteins. An extensive research of quantitative and qualitative analysis will bring in more perspective on lipoprotein as important biomarkers of CAD. In this study, HDL and LDL particles in blood plasma of ten CAD patients and a control group of ten normal people were separated by an effective method of multiplexed hollow fiber flow field-flow fractionation (MxHF5) with an advantage of its ability to facilitate the separation significantly fast with substantial amount of samples. Among the three different extraction methods - Folch, HLB cartridge, and methyl tert-Butyl ether - the method of Folch provided the highest efficiency; the samples were extracted by the method of Folch. Phospholipids along with lysophospholipids in the extracted HDL and LDL samples were quantitatively and qualitatively analyzed using a nanoflow liquid chromatography electrospray ionization tandem mass spectroscopy (nLC-ESI-MS-MS).

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장소: 제주ICC

발표코드: IV-ANAL.P-15

발표분야: 분석화학

발표종류: 포스터, 발표일시: 금 15:00~17:00

## Improvement of Lipoprotein Separation in Asymmetrical Flow Field-Flow Fractionation with Guard Channel & Fluorescence Detection

이주용, 문명희

연세대 화학과

Low density lipoprotein (LDL), among the lipoprotein classes, is known as a critical factor in coronary artery disease (CAD). Especially, presence of small, dense low-density lipoproteins (LDL) is associated with cardiovascular risk. A few studies reporting the relationship between CAD and LDL sizes and concentration by flow field-flow fractionation (FIFFF) have been reported [1,2]. A relatively large amount of serum proteins (approximately 60  $\mu\text{g}/\mu\text{L}$  serum) existent in a small amount of serum causes a problem by contaminating and blocking the pores of a membrane in FIFFF channel, which leads to a fluctuation of retention times in repeated runs. In this study, a guard channel prior to an asymmetrical FIFFF (AFIFFF) channel and a fluorescent phospholipid dye are used for to improve the reproducibility of lipoprotein separation. The guard channel was made of a simple hollow fiber module so that the serum sample can be washed with the help of radial flow prior to injection into the AFIFFF channel. A fluorescent dye was applied to label lipoprotein particles before injection to the AFIFFF channel, which resulted in a reduction of the minimum volume for lipoprotein detection.[1] I. Park, K.-J. Paeng, D. Kang, M.H.Moon, J. Separation Sci. 28 (2005) 2043-2049[2] I. Park, K.-J. Paeng, Y. Yoon, J.-H. Song, M. H. Moon, J. Chromatogr. B. 780 (2002) 415-422

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장소: 제주ICC

발표코드: IV-ANAL.P-16

발표분야: 분석화학

발표종류: 포스터, 발표일시: 금 15:00~17:00

## Characterization of Hydroxyethyl Starch and Its Blended Mixture with Sodium Hyaluronate by Flow Field-Flow Fractionation and Multi-angle Light Scattering

무하마드 알리, 문명희

연세대 화학과

Hyaluronan or hyaluronic acid (HA) is a natural polysaccharide with a disaccharide repeating unit, [(1 → 3)-O-(2-acetamido-2-deoxy-β-D-glucopyranosyl)-(1 → 4)-O-β-D-glucopyranuronosyl]. HA is found naturally in the skin, synovial fluid, umbilical cord, vitreous humor, human cartilage, and rooster comb, and can also be obtained using microbiological methods. HA is utilized as a sodium salt of hyaluronic acid (NaHA) and it has versatile uses in ophthalmic surgery, arthritis treatment, wound repair, and cosmological applications, due to the biologically safe nature and characteristic properties of the material. In this study, differently blended films of hydroxyethyl starch (HES) with NaHA and poly(lactic-co-glycolic acid) (PLGA) were examined. These films can be utilized as anti-adhesive in abdominal surgery. Analytically efficient Frit Inlet Asymmetric Flow Field Flow Fractionation (FIAFFFF) along with Multi-angle light scattering/differential refractive index detector enabled us to elucidate information about their size, molar mass distribution, and conformation. For the sake of control we analyzed NaHA+HES blended mixture. Molar masses of the samples were found to be in the range of 10<sup>5</sup> to 5×10<sup>7</sup>g/mole. Relationship between molecular weight and root mean square radius disclosed no distribution of molecules higher than the constituents. Thus, blended mixture of HES with NaHA and PLGA did not cause any aggregation effect. It showed to have both compact and linear molecules in its molecular distribution making available of comparing the slope values for linear structure molecules in blended mixture samples. Moreover, no aggregation could be seen either in NaHA+HES+PLGA film products or in NaHA+HES blended mixture.

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장소: 제주ICC

발표코드: IV-ANAL.P-17

발표분야: 분석화학

발표종류: 포스터, 발표일시: 금 15:00~17:00

## Fractionation of Phosphorylated Proteins by Isoelectric Focusing and Flow Field-Flow Fractionation

김기훈, 문명희

연세대 화학과

Phosphorylation of protein plays a critical role in cell signaling and other fundamental cellular functions in living organisms. It has been reported that phosphorylation of a protein is involved with some diseases. Therefore, it is of interests to develop a noble method to separate phosphorylated proteins by the degree of phosphorylation for clinical applications. In this poster, it will be introduced with a recent development of a non-gel based high speed two-dimensional protein separation devices based on the on-line combination of Isoelectric Focusing (IEF) and asymmetrical flow field-flow-fractionation (AF4). This system is able to separate proteins by the differences of pI value and Stoke's diameter (size-based separation) without using gel or stationary phase within 30 minutes. When IEF-AF4 system was applied for the 2D fractionation of phosphorylated proteins, it requires an ampholyte with very narrow pH range (~0.5) and therefore the ampholyte solution for the specific needs was prefractionated with IEF channel in the lab. For the performance test of IEF-AF4 for phosphorylated proteins, it was demonstrated with the separation of  $\alpha$ -casein by different number of phosphorylation at different channel lanes of AF4 and the degree of phosphorylation was determined by comparing the peak area at each lane. The fractionated phosphoproteins were analyzed by nanoflow LC-ESI-FTICR-MS after tryptic digestion. From the database search, it was found that four phosphorylated peptides of  $\alpha$ -casein fractions were identified according to the different pI values and that each peak area of phosphopeptide increased with the decrease of pH.

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장소: 제주ICC

발표코드: IV-ANAL.P-18

발표분야: 분석화학

발표종류: 포스터, 발표일시: 금 15:00~17:00

## Evaluation of three common kinds of microalgae in Korea for biodiesel production

여인준, 정지은, 조윤주, \*김성홍, 김성환

경북대 화학과 \*한국기초과학지원연구원 대구분소

Microalgae have been suggested as good candidates for fuel production because of their advantages of higher photosynthetic efficiency, higher biomass production and faster growth compared to other energy crops. One of the major bottlenecks of algae biodiesel production is low efficiency in converting algae to biodiesel. To improve the production efficiency, it is very important to understand the compositions of fatty acids in algae of interest. Algal biodiesel is mainly composed of a mixture of unsaturated fatty acids: palmitoleic acid (C16:1), oleic acid (C18:1), linoleic acid (C18:2) and linolenic acid (C18:3). Saturated fatty acids such as palmitic (C16:0) and stearic (C18:0) are also present in microalgae although to a small extent. However, it should be noted that the fatty acid composition varies greatly depending on each algal species. In this study, significant amounts of heptadecane and hexadecenol in algal biodiesel produced by *Nostoc sp.* were observed by GC-MS analysis. Thus, the aim of this study is to isolate and identify algal strains possibility of producing fuel which may be modified to produce biodiesel.

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장소: 제주ICC

발표코드: IV-ANAL.P-19

발표분야: 분석화학

발표종류: 포스터, 발표일시: 금 15:00~17:00

## Enhanced chemical characterization of heavy crude oil samples by combination of high resolution mass spectrometry and SARA fractionation

조윤주, \*김성홍, 김성환

경북대 화학과 \*한국기초과학지원연구원 대구분소

Fourier transform ion cyclotron resonance mass spectrometry (FT-ICR MS) coupled to atmospheric pressure photo ionization (APPI) has been successfully used for characterization of heavy crude oils at the molecular level. However, crude oil contains such an extensive range of compounds that a complete analysis of chemicals is not trivial. One of the problems is that matrix effect and ionization suppression can limit number of chemicals observed by FT-ICR MS. In this study, heavy crude oil samples were fractionated by a widely used Saturates/Aromatics/Resins/Asphaltenes (SARA) fractionation method before FT-ICR MS analysis. Each SARA fractions extracted from bitumen and Arabian heavy crude oil were compared. Bitumen is determined to be heavier than ARH because bitumen contained more proportion of resins and asphaltene content. The SARA fractionation separates the crude oil into four main classes based on polarity and solubility. Subsequent FT-ICR MS analysis of each fraction yielded spectrum which was quite different from one obtained from unfractionated crude oil. As a result, more than two times the number of chemicals could be identified after combining SARA fractionation and APPI FT-ICR MS. For example, numerous NO<sub>x</sub> and SO<sub>x</sub> class compounds which were not observed in the direct analysis of unfractionated heavy crude oils were abundant in resin fraction. More S class compounds presumably with thiol group were observed. By the combined approach, more than 20,000 peaks were routinely identified from a single crude oil samples. So, even minor components of crude oil could be detected by this combined approach. Standard compounds were synthesized and added to each fraction for more quantitative comparison. Spectra with the same standard/sample ratio were compared and it was clear that ionization efficiencies were vastly different from fraction to fraction. Saturate fraction presumably the lightest fraction had the highest ionization efficiency. However, resin and



asphaltene fractions had much lower ionization efficiency. Overall, this study shows that it is necessary to combine chromatographic techniques including fractionation with high resolution mass spectrometry for more complete understanding of heavy molecules comprising petroleum.



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장소: 제주ICC

발표코드: IV-ANAL.P-20

발표분야: 분석화학

발표종류: 포스터, 발표일시: 금 15:00~17:00

## **Molecular level characterization and evaluation of shale oils generated by different pyrolysis methods**

진장미, 김성환

경북대 화학과

In this research, shale oils were analyzed by use of the Fourier transform ion cyclotron resonance mass spectrometry (FT ICR-MS) combined with electrospray ionization (ESI) and atmospheric pressure photoionization (APPI). Shale oils were produced from Eocene Green River Mahogany zone oil shale by three pyrolysis methods with various temperature and extraction times. The class and double-bond equivalence (DBE) distributions of shale oils were obtained from spectra, and were compared. As a result, Nx classes compounds were mostly abundant in shale oils. It was observed that relative abundance of Nx compounds and DBE distributions could vary significantly by use of different pyrolysis methods. DBE distribution showed that molecular structures of compounds could also change depending on the extraction conditions. This study clearly shows that high resolution mass spectrometry can provide detailed chemical information that can be useful in developing efficient shale oil extraction method.

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장소: 제주ICC

발표코드: IV-ANAL.P-21

발표분야: 분석화학

발표종류: 포스터, 발표일시: 금 15:00~17:00

## Antibody Coated Gold Nanocubes for QCM and SPR Analysis of Protein Biomarkers

남은지, 김엄지, 이혜진

경북대 화학과

This poster demonstrates a highly sensitive detection method for protein biomarkers using antibody functionalized gold nanocubes in conjunction with quartz crystal microbalance (QCM) and surface plasmon resonance (SPR). As a model protein biomarker, immunoglobulin E (IgE) is selected because the protein has two different binding sites, anti- IgE and IgE specific aptamer, allowing us to design a sandwich detection format without the need of labeling the target protein. The sandwich complex is formed via the adsorption of IgE onto the surface bound IgE-aptamer followed by the adsorption of anti-IgE coated gold nanocubes. A robust and reproducible cross-linking chemistry for the attachment of antibodies onto Au nanocubes is developed using a carboxylic acid terminated alkane thiol and a combined use of 1-ethyl-3-(3-dimethylaminopropyl)carbodiimide (EDC) and N-hydroxysulfosuccinimide (NHSS). Gold nanocubes coated with antibodies are then characterized with UV-vis spectroscopy and TEM. The sequential adsorption of IgE and anti-IgE coated Au nanocube on the IgE-aptamer immobilized on a poly(ethylene glycol) modified gold surface is monitored in-situ using both QCM and SPR. All results for IgE sandwich assays from both detection techniques utilizing the same gold surface functionalization chemistry were thoroughly compared and analyzed.

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장소: 제주ICC

발표코드: IV-ANAL.P-22

발표분야: 분석화학

발표종류: 포스터, 발표일시: 금 15:00~17:00

## Enhanced SPR Detection for Proteins with Biofunctionalized Gold Nanocages and Aptamer chips

권민정, 김엄지, 김성엽, 이해진

경북대 화학과

A highly sensitive SPR detection method for proteins in conjunction with biofunctionalized gold nanocages and an aptamer chip is demonstrated. As a model protein, thrombin (Th) which is an important anticoagulant was selected since the protein has two different epitopes for an anti-Th and a thrombin specific aptamer (Th-apatmer) allowing a label-free detection configuration forming a surface sandwich assay platform. The surface sandwich complex was created via the adsorption of thrombin on Th-aptamer molecules immobilized on a prolinker B modified gold surface followed by the adsorption of anti-Th coated gold nanocages on the surface thrombin/Th-aptamer complex. The attachment of Th-aptamer via prolinker B linker on a gold surface was first characterized using PM-FTIRRAS and AFM. The direct SPR detection of thrombin in conjunction with anti-Th coated gold nanocages and Th-apatmer chip was then monitored in real-time. The use of biofunctionalized gold nanocages with an aptamer chip could enhance the SPR detection limit down to ~ fM concentration of protein molecules.

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장소: 제주ICC

발표코드: **IV-ANAL.P-23**

발표분야: 분석화학

발표종류: 포스터, 발표일시: 금 15:00~17:00

## **Immunosensing of Tuberculosis CFP-10 based on SPR Spectroscopy**

홍성철, 이재범

부산대 나노메디컬공학과

An antigen (Ag), CFP-10, found in the urine of Tuberculosis(TB) patients may be an ultimate candidate for use as a sensitive TB marker with a sensing method for early simplified diagnosis of TB. In this study, chemical and optical optimizations were carried out using novel immuno-materials for establishment of a self-assembled surface plasmon resonance (SPR) optical immunosensor system for detection of CFP-10, which is valuable for pre-clinical work, prior to conduct of massive clinical observations. For creation of a simple sensing interface, a single-chain variable fragment (scFv) monoclonal antibody (anti-CFP-10) was immobilized directly on a gold surface, followed by blocking with cystamine. Orientation and accessibility of anti-CFP-10 were assessed by the selective binding of CFP-10. Recent results indicate that the reusability of the sensor chip adopting the cystamine method was found to be preferable to other immobilization methods. A linear relationship was well correlated between SPR angle shift and CFP concentrations in the range from 0.1 to 1 g mL<sup>-1</sup>. Modification of the SPR chip with scFv antibody provides a simple experimental platform for investigation of isolated proteins under experimental conditions resembling those of their native environment. Therefore, it is believed that with further clinical case studies, immunological analysis using CFP-10 can be a promising tool for use with a reliable and robust sensing system for TB diagnosis.

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장소: 제주ICC

발표코드: IV-ANAL.P-24

발표분야: 분석화학

발표종류: 포스터, 발표일시: 금 15:00~17:00

## The stability of copper with hydrotalcite by deposition, using electrolysis

김태호, 김지혜, 나성욱, 김종원, 정용석, 권수한

충북대 화학과

본 연구는 전기분해를 이용하여 하이드로탈사이트에 구리이온을 침착시키는 것을 목적으로 한다. 전기분해 장치를 이용해 구리판에서 구리이온을 얻어 침착시키는 것으로 반응시간, 온도, pH, 전압을 변화시켜 반응성을 알아보고 나타난 결과를 보고 반응이 일어나는 최적조건을 찾는다. 그 생성된 물질과 기존 물질의 안정성을 테스트해보고 유용한 물질을 찾아낸다. 또한 향균성을 측정해 다른 유용한 물질로 사용될 수 있을지 연구한다. 본 연구는 교육과학기술부와 한국산업기술재단의 지역혁신인력양성사업으로 수행된 연구결과임.

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장소: 제주ICC

발표코드: IV-ANAL.P-25

발표분야: 분석화학

발표종류: 포스터, 발표일시: 금 15:00~17:00

## Investigation of an unanticipated peak caused by DHB-Pyridine ionic matrix using MALDI-TOF MS

홍장미, 이선영, 김재현, 김정권

충남대 화학과

Numerous matrices are used for analysis of numerous samples by matrix-assisted laser desorption/ionization time-of-flight mass spectrometer (MALDI-TOF MS). Solid matrices are usually used as a MALDI matrix. However, one of the most problems by convectional matrices such as dihydroxybenzoic acid (DHB),  $\alpha$ -cyano-4-hydroxycinnamic acid (CHCA) or sinapinic acid (SA) is the formation of heterogeneous sample spots. The matrices make the quantification of analyte using MALDI system difficult. To reduce the problem of these matrices, the use of ionic liquids has been introduced as MALDI matrices in recent years. Various ionic liquid matrices (ILMs) have been used for the analysis of samples in MALDI-MS. In this study, we characterized a particular peak at  $m/z$  232.1 originated from a ILM of DHB-Pyridine. The ILM is made by dissolving pyridine with DHB at a molar ratio of 1:1. To confirm the peak from this ILM, a extensive study has been performed with various DHBs such as 2,3-DHB, 2,4-DHB, 2,5-DHB, 2,6-DHB, 3,4-DHB and 3,5-DHB mixed with pyridine. It is found that the peak was only shown from 2,3-DHB and 2,5-DHB. Additionally, we propose a mechanism for the formation of  $m/z$  232.1 peak.

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장소: 제주ICC

발표코드: **IV-ANAL.P-26**

발표분야: 분석화학

발표종류: 포스터, 발표일시: 금 15:00~17:00

## **Analysis of chitooligosaccharides using LC-MS/MS**

김재현, 홍장미, 이선영, 박세환, 김정권

충남대 화학과

Chitooligosaccharide is a kind of oligosaccharide which is made from chitin or chitosan through chemical or enzymatic decomposition. In this study, reversed-phase high-performance liquid chromatography (HPLC) combined with electrospray ionization (ESI) quadrupole ion trap mass spectrometry was utilized for the characterization of chitooligosaccharide. ESI is a powerful ionization technique for structural elucidation of oligosaccharides. In HPLC, a polymer-based amine column is used to separate the isomers of chitooligosaccharides where isocratic elution with 75% acetonitrile (ACN) in water was used to elute out sample from the amine column. The standard and real samples of chitooligosaccharide were prepared in a concentration of 30 mg/mL in water. The isomer of chitooligosaccharide was effectively separated using the amine column and fragmented in a ion trap analyzer providing sequence information of each isomer. The detailed experimental procedures and results will be provided during the presentation.



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장소: 제주ICC

발표코드: IV-ANAL.P-27

발표분야: 분석화학

발표종류: 포스터, 발표일시: 금 15:00~17:00

## Comparison of different tryptic digestion methods in the analysis of bovine plasma proteins

박세환, 홍장미, 이선영, 김재현, 김정권

충남대 화학과

Generally, using overnight tryptic digestion of proteins requires over 12 hour. Recently, several different digestion methods were introduced to expedite the digestion. In this study, we aim to find the most efficient tryptic digestion method. The performance of five different digestion methods (Overnight, Microwave, Ultrasound, Vortex and Pressure) used in the tryptic digestion of bovine plasma proteins was compared by using electrophoresis. The plasma sample was prepared in a concentration of 10 mg/ml. Denaturation of plasma sample was accomplished with 6M Guanidine HCl. Reduction and alkylation were performed by adding dithiothreitol and iodoacetamide, respectively. The plasma sample was then divided into two portions. One portion was directly digested by using one of the five different methods, while the other portion was filtered by using a YM-10 filter to remove any salts in the sample and then digested by using one of the five different methods. Conventional overnight tryptic digestion was performed for 12 hour at 37°C. Microwave-assisted tryptic digestion was performed for 10 min or 1 hour. Ultrasound-assisted, vortex-assisted and 6 atm pressure-assisted tryptic digestions were performed for 10 min or 1 hour at 37°C or 55°C.

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장소: 제주ICC

발표코드: IV-ANAL.P-28

발표분야: 분석화학

발표종류: 포스터, 발표일시: 금 15:00~17:00

## **Analysis of mono-sugars obtained by acid hydrolysis of algae-based polysaccharides**

**강은경, 황현아, \*김지현, \*\*박종목, \*\*강호철, \*\*이병민**

과학기술연합대학원대 청정화학및 생물학전공 \*충남대 바이오응용화학 \*\*한국화학연구원 그  
린화학연구단

Fossil fuel reserves are limited and global warming is emerging as a serious problem. To solve these problems, efforts to develop alternative energy sources are underway. In recent years the chemical industry based on the environmentally sound and sustainable biomass has been developing. Polysaccharides such as cellulose and galactan obtained from the biomass can be converted to simple mono-saccharides by acid hydrolysis reactions. The formed monosaccharides are analyzed quantitatively and qualitatively by using liquid chromatography, ion chromatography and gas chromatography. By using acids to hydrolyze polysaccharides, monosaccharides can be formed as the structure of close form and/or open form. In this study, analysis methods of monosaccharides formed by acid saccharification are investigated to distinguish between close form and open form.

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장소: 제주ICC

발표코드: IV-ANAL.P-29

발표분야: 분석화학

발표종류: 포스터, 발표일시: 금 15:00~17:00

## Fast extraction method of human nail proteins using microwave

이선영, 홍장미, 박세환, 김재현, 김정권

충남대 화학과

Traditional extraction method of human nail protein is very time consuming. In this study, we investigate fast extraction method of human nail protein using microwave radiation (600 W). Nail samples (2 mg) in an extraction solution composed of 25 mM Tris-HCl (pH 8.5), 2.6 M thiourea, 5M urea, and 5% mercaptoethanol are incubated for a certain duration ranging from 5 min to 120 min. Extracted proteins are analyzed by sodium dodecyl sulfate-polyacrylamide gel electrophoresis (SDS-PAGE). For quantitative analysis, Bradford method is used where BSA standard and 20 times diluted proteins are mixed with Coomassie Plus Reagent solution in microplate wells, incubated for 10 min at room temperature and was absorbance measured at 595 nm. Compared to traditional extraction method, this novel extraction method using microwave provided similar extraction efficiency with reduced extraction time.

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장소: 제주ICC

발표코드: IV-ANAL.P-30

발표분야: 분석화학

발표종류: 포스터, 발표일시: 금 15:00~17:00

## Compact Continuous-Flow PCR System

김한옥, 곽병주, 한종훈

포항공과대 화학과

We have developed a compact continuous-flow PCR device fabricated only from solid components and demonstrated the possibility of high-throughput PCR amplification in a segmented-flow mode. The device performs PCR by having a reaction solution flow through a long capillary wound helically around a cylindrical thermal cyclor with a fixed pitch per turn of the helix. Three thermally insulated metal heating blocks are arranged to form the cylindrical structure and run thermal cycles repetitively, in the sequence of melting, annealing, and extension. Since there is an air gap between the extension and melting blocks, the parallel, bridging parts of the capillary can be severed as windows of laser-induced fluorescence (LIF) detection for quantitating a DNA product during the course of amplification in real-time PCR. The cylindrical continuous PCR device can be applicable in optimization-free PCR that could set different annealing temperatures at each four station, thus possible to use for rapidly determine the optimum PCR condition of different samples, using a minimal amount of reagents and time. This miniaturized continuous PCR device also can be interfaced with the capillary electrophoresis (CE) microchip for on-line analysis of the DNA fragment. This microchip is for sequential high-throughput analysis of different amplified DNA product and the analysis is contamination-free method that can collect pure PCR products by separating with DNA analysis process using intercalating dye.

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장소: 제주ICC

발표코드: IV-ANAL.P-31

발표분야: 분석화학

발표종류: 포스터, 발표일시: 금 15:00~17:00

## Selective Screening of Tyrosine-Nitrated Peptides in Tryptic Mixtures by In-Source Photodissociation at 355 nm in Matrix-Assisted Laser Desorption Ionization

신영식, \*문정희, 김명수

서울대 화학부 \*한국생명공학연구원 단백질의학연구센터

Nitration of tyrosine residues in proteins is an important post-translational modification related to various diseases such as Alzheimer's. In this work, efficient and selective photodissociation (PD) at 355 nm was observed for  $[M + H]^+$ ,  $[M + H - 16]^+$ , and  $[M + H - 32]^+$  generated by matrix-assisted ultraviolet laser desorption ionization (UV-MALDI) of tyrosine-nitrated peptides (nitropeptides). Product ion spectra obtained by post-source PD at this wavelength contained useful information on amino acid sequence. The spectra for nitropeptides obtained with 355 nm irradiation inside the ion source (MALDI/in-source PD) displayed characteristic triplet patterns due to PD of the above ions. For peptides displaying prominent signal in MALDI mass map of a tryptic mixture, which are mostly those with arginine at the C-terminus, in-source PD allowed positive identification of their tyrosine-nitrated forms. Identification of such nitropeptides was possible at the 10 fmol level (in tryptic digest of 100 fmol BSA).

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장소: 제주ICC

발표코드: IV-ANAL.P-32

발표분야: 분석화학

발표종류: 포스터, 발표일시: 금 15:00~17:00

## Microchip-Based System for Monitoring Chromium in Water

안재훈, 조경호, 한종훈

포항공과대 화학과

We have developed a microchip-based analysis system for a continuous monitoring of Cr(III) and total chromium with chemiluminescence detection. The microchip is fabricated with black poly(dimethylsiloxane)(PDMS) which can block the stray light and decrease the noise. The 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). Cr(III) can be quantitatively determined by measuring the light emission. By selective injection of the reductant, we can determine the total chromium and Cr(III). Cr(VI) is calculated by the difference between total chromium concentration and that of Cr(III). The potential interference effect by other metal ions is quenched by adding EDTA to form complexes that are not active as catalysts.

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발표분야: 분석화학

발표종류: 포스터, 발표일시: 금 15:00~17:00

## Amperometric Tyrosinase Biosensor Based on Graphene Doped Sol-Gel-Derived TiO<sub>2</sub>-Nafion Composite Films

김자영, 최한님, 이원용

연세대 화학과

Graphene offers excellent electronic, thermal and mechanical properties. And graphene from reduction of graphene oxide has abundant defects and functional groups which are advantageous for electrochemical applications. In this study, we developed a highly sensitive amperometric tyrosinase biosensor based on mesoporous composite films of RGON(reduced graphene oxide with Nafion intercalation)-TiO<sub>2</sub>-Nafion composite film encapsulating tyrosinase on a glassy carbon electrode. Surface characters of RGON are tested by several physical methods such as FT-IR, Raman, and XPS to confirm synthesis of RGON. Due to the high surface and high conductivity of graphene, the biosensor has excellent electrocatalytic activity, facilitated electron transfer, and low interfacial resistance. Therefore, this present biosensor exhibits very faster response time, higher sensitivity, and lower detection limit for phenol than those obtained with the conventional biosensor based on carbon nanotube-TiO<sub>2</sub>-Nafion composite film. Furthermore, it is expected that the present biosensor can be employed to the determination of phenolic compounds in real samples such as industrial waste water.

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장소: 제주ICC

발표코드: IV-ANAL.P-34

발표분야: 분석화학

발표종류: 포스터, 발표일시: 금 15:00~17:00

## Electrochemical Determination of Hemoglobin A<sub>1c</sub>

성기영, 최한님, 이원용

연세대 화학과

The amount of Hemoglobin A<sub>1c</sub> can be a indicator for average blood glucose level over the 2-3 months. Therefore, Hemoglobin A<sub>1c</sub>, glycated hemoglobin is the dependable indicator for the long-term management of diabetic. In this study, the amount of Hemoglobin A<sub>1c</sub> is measured by using the label-free electrochemical detection based on the specific cis-diol interaction of Hemoglobin A<sub>1c</sub> with boronic acid. Detection of Hemoglobin A<sub>1c</sub> was performed with simple procedure. First of all, Hemoglobin A<sub>1c</sub> was specifically bound to the boronic acid-modified self-assembled monolayer on gold electrode. And then, ferrocene boronic acid derivatives were bound to the opposite binding site of Hemoglobin A<sub>1c</sub>. The concentration of Hemoglobin A<sub>1c</sub> was determined by measuring the cyclic voltammetric response of the bound ferrocene boronic acid derivatives. Self-assembled monolayers with different chain length were tested to bring out enhancement in electrical signal. Also, we introduced several kinds of ferrocene boronic acid derivatives to find out the molecule which gives the enhanced signal. In addition, we modified the self-assembled monolayers with poly(ethylene glycol) moieties to prevent non-specific protein adsorption. Furthermore, the present Hemoglobin A<sub>1c</sub> sensor will be tested with real human blood for practical applications.



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발표분야: 분석화학

발표종류: 포스터, 발표일시: 금 15:00~17:00

## Single protein picking by atomic force microscopy

김덕희, 박준원

포항공과대 화학과

A cone shaped dendron modified surface has provided ample lateral spacing and enabled us to investigate single molecular interactions. The modification with dendron also realized single DNA picking up and single new DNA introduction at the apex of AFM tips. This approach was expanded to the picking up of a single protein molecule. Single protein picking up was confirmed by TEM imaging, and further application of the tip was also investigated.

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발표분야: 분석화학

발표종류: 포스터, 발표일시: 금 15:00~17:00

## **Judgement of signature made with ballpoint pen ink on illegal and counterfeit documents using Micro-Attenuated Total Reflectance FTIR spectroscopy**

남윤식, 박현미, 이강봉

KIST 특성분석센터

Ballpoint pen ink signatures on questioned documents were studied to investigate the feasibility of micro-Attenuated Total Reflectance (ATR) FTIR spectroscopy as a tool in the forensic study. Micro-ATR FTIR spectra for signatures made with ballpoint pens available commercially in Korea were collected and analyzed. The technique was able to differentiate black ballpoint pen inks of different brands or manufacturers. Blind testing for discrimination of the ballpoint pen signatures has shown that micro-ATR FTIR can accurately discriminate the origin and fake of ballpoint pen ink used for signature. Data gathered were stored to use a spectral database for future reference. The results show that micro-ATR FTIR can be a valuable non-destructive tool for the objective analysis of questioned documents involving ballpoint pen ink signature. It could an objetive method of analysis that is based on chemical differences of inks inherent to the sample involved.

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발표분야: 분석화학

발표종류: 포스터, 발표일시: 금 15:00~17:00

**Revelment of non heterogeneous nature of oxygenated compounds in  
dissoved organic matter: observation and application of linearity  
between average double bond equivalence, carbon number and  
number of oxygen**

김병준, 배은정, 김성환

경북대 화학과

Dissolved organic matter was studied by high resolution mass spectrometry and it was observed that there existed strong linear relationship between average double bond equivalence and average carbon number vs number of oxygen atoms in oxygenated compounds. The compounds were observed by negative mode electrospray ionization coupled to Fourier transform ion cyclotron resonance mass spectrometry. The slope and intercept of the linear relationship compounds are shown to be useful for comparison of DOM. For coast offshore DOM molecules, the addition and removal of two oxygen atoms resulted in difference of double bond equivalence (DBE) by 1. Inland riverine samples had DBE difference of 1.5 per two oxygen atoms. The extra change in DBE of inland riverine sample can be attributed to presence of unsaturated chemical bonds and cyclic structure. The result presented in this study clearly shows that oxygenated compounds in DOM may not be heterogeneous. It also shows that the observed linearity can be effectively used to compare structure difference between DOM samples.

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발표종류: 포스터, 발표일시: 금 15:00~17:00

## **Influence of UV stabilizer on MALDI-MS analysis of PEG and PS**

정혜승, 최성신

세종대 화학과

In analysis of matrix-assisted laser desorption/ionization-mass spectrometry (MALDI-MS), matrix absorbs UV radiation and then delivers energy to an analyte. For using N<sub>2</sub> laser (337nm) as a light source, matrices have to absorb UV of 337nm. In MALDI analysis of polyethylene glycol (PEG) and polystyrene (PS), general matrices are 2,5-dihydroxybenzoic acid (DHB), retionic acid and dithranol. Ultraviolet light absorber (UVA) and ultraviolet light stabilizer (UVS) are used in polymeric materials for preventing them from degradation by UV radiation in sunlight. Because UVA absorbs UV radiation of 337nm, it is going to role as matrix in MALDI. In this study, we applied UVA and UVS as matrix for analysis of PEG and PS. It was found that UVA and UVS enhanced ionization efficiencies of PEG and PS.

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발표종류: 포스터, 발표일시: 금 15:00~17:00

## Formation of $[M+anion]^-$ of explosives in APCI-MS

김옥배, \*최성신, \*\*신명원, \*\*최규섭, \*\*맹석진, \*\*안승건

세종대 응용화학과 \*세종대 화학과 \*\* (주)우주씨앤티 기술연구소

Explosives are unstable compounds and their polarity varies from moderate to high due to their nitro groups. These properties impose certain limitations on techniques used for their analysis, since explosives may be decomposed during the analysis or result in poor chromatographic retention. Gas chromatography mass spectrometry (GC/MS) is suitable for the analysis of nitroaromatic compounds, but not for nitrate esters and nitroamines, which undergo thermal decomposition under these conditions. And time-of-flight mass spectrometry (TOFMS) is suitable for the analysis of explosives, but reproducibility and sensitivity are insufficient. Liquid chromatography/mass spectrometry (LC/MS) would be a better alternative for the more unstable and polar explosives. Atmospheric pressure chemical ionization (APCI) applies mild ionization for the analysis without destroying the sample. APCI is a useful ionization for analysis of explosives such as pentaerythritol tetranitrate (PETN) and 1,3,5-trinitroperhydro-1,3,4-triazine (RDX). In this study, the explosives were analyzed with APCI-MS and formation of the  $[M+anion]^-$  were examined. The  $[M-H]^-$ ,  $[M+Cl]^-$ ,  $[M+NO_2]^-$ , and  $[M+NO_3]^-$  ions were observed. Chlorine-donating compounds and nitrate-donating compounds were employed as dopants to generate the  $[M+anion]^-$ .

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발표코드: IV-ANAL.P-40

발표분야: 분석화학

발표종류: 포스터, 발표일시: 금 15:00~17:00

## Direct Observation of Real-Time Enzymatic Digestion of Single-DNA Molecule

이승아, 강성호

경희대 응용화학과

Single-DNA molecule digested by enzyme was directly observed with real time by dual-color total internal reflection fluorescence microscopy. DNA molecules intercalated with the fluorescent dye (bp:dye = 50:1) were stretched on a fused-silica prism surface. Enzyme digestion was initiated by the influx of exonuclease. The DNA digestion rates of enzyme based on the decreasing of length showed three digestion types. The digestion rates were also compared to the ensemble averaged data obtained in the bulk solution by capillary electrophoresis.

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발표종류: 포스터, 발표일시: 금 15:00~17:00

## A study about Ni-hydrotalcite synthesis as high functional and active plastic additives

나성옥, 김종원, 정용석, 권수한

충북대 화학과

충상 이중 수산화물인 하이드로탈사이트는 두 층 사이로 음이온을 포획하는 우수한 기능을 가지고 있다. 다양한 종류의 수지에 여러 다른 첨가제와 함께 사용되어 수지의 물성의 개선 및 안정성을 향상시킬 수 있다. 본 연구는 니켈금속의 전기분해를 통하여 니켈을 하이드로탈사이트 표면에 침착시킴으로써 하이드로탈사이트와 촉매제를 따로 사용할 필요없이 한 번에 사용 가능한 고기능 고효능 플라스틱 첨가제에 대해 연구하는데 있다. 본 연구는 교육과학기술부와 한국산업기술재단의 지역혁신인력양성사업으로 수행된 연구결과임

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장소: 제주ICC

발표코드: IV-ANAL.P-42

발표분야: 분석화학

발표종류: 포스터, 발표일시: 금 15:00~17:00

## Cation Effect on DNA Base Stacking in Capillary Electrophoresis

신아람, \*강성호

경희대 대학원 화학과 \*경희대 응용화학과

Effect of cations on base stacking (BS) was investigated for high sensitive detection of DNA fragments in capillary electrophoresis (CE). BS method was achieved simply by electrokinetic injection of hydroxide ion ( $\text{OH}^-$ ) after DNA sample injection. Neutralization reaction was occurred between the hydroxide ions region and running buffer component  $\text{Tris}^+$  region, which resulted in a zone of lower conductivity. Within the low conductivity zone of high electric field, the DNA fragments more rapidly moved than that in untreated buffer zone. For the effective BS, the optimum condition was determined by altering the concentration of NaOH (0.05 - 1.50 M) and injection time (0 - 210 s) under various cationic hydroxides (i.e.,  $\text{NH}_4^+$ ,  $\text{K}^+$ ,  $\text{Mg}^{2+}$  and  $\text{Ca}^{2+}$ ). The BS method will be a pre-concentration technique for the high sensitive detection of DNA fragments in CE.



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발표분야: 분석화학

발표종류: 포스터, 발표일시: 금 15:00~17:00

## Multi-Channel Microchip Electrophoresis for High-Throughput Screening of DNA Fragments

Nan He, \*강성호

경희대 대학원 화학과 \*경희대 응용화학과

Home-made multi-channel microchip electrophoresis (MC-ME) system with a laser induced fluorescence detector was investigated for high-throughput screening of DNA fragments. Although microchip electrophoresis (ME) is characterized as a fast and effective separation method, conventional ME allows the analysis of only one sample at a time. For simultaneous detection of DNA fragments, multi-channel microchip was fabricated with three channels to analyze different samples in parallel. Separation was achieved with a sieving matrix of poly(ethylene oxide) ( $M_r = 8\,000\,000$ ) in  $1\times$  TBE Buffer. This work established the feasibility of using the MC-ME system for high-speed, high-throughput DNA analysis of different samples.

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발표종류: 포스터, 발표일시: 금 15:00~17:00

## Visualizing Hydrodynamic Behavior of the Surface-immobilized DNA using AFM Force Spectroscopy

이윤희, 박준원

포항공과대 화학과

Force-mapping mode of atomic force microscopy (AFM) is widely used to study the distribution of biomolecules located on cell membranes. To detect the target molecules using this technique, the specific adhesion forces are measured by the functionalized tip, moving above the surface with sub-nanometer spatial resolution. Therefore, the spatial distribution of target molecules could be mapped by analyzing adhesion forces. Based on the force-mapping technique, we visualize the hydrodynamic behavior of the surface-immobilized single strand DNA. Using dendron-coated surface, which guarantee mesospacing, we could recognize individual DNAs on surface with the complementary DNA on AFM tip. The target DNA has characteristic dynamic radius on surface according to its length. As a result, the hydrodynamic behavior could be printed on the high resolution force map. This study enhances our knowledge about the mechanical properties of the surface-immobilized DNA. Moreover, it could be attributed to the development of the force-based single DNA detection method.

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발표종류: 포스터, 발표일시: 금 15:00~17:00

## Single metal nanoparticle attachment at the apex of an AFM tip

김웅, 김덕희, 박준원

포항공과대 화학과

We reported the generation of a novel meso spaced surface prepared by applying dendron molecules on the solid surface. Dendron modified surface has been shown to outstandingly perform the picking of a single metal nanoparticle. Through the picking of a single metal nanoparticle, a single metal nanoparticle is attached to the edge of AFM tip. A single metal attached to AFM tip was confirmed by TEM imaging. We will strongly use a single nanoparticle's characteristic for bioassays and these methods will be possible to various applications of nanomaterial field.

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발표종류: 포스터, 발표일시: 금 15:00~17:00

## Hydrodynamic Behavior of Surface-conjugated A $\beta$ Observed by AFM Force Spectroscopy

김영규, \*박준원

포항공과대 시스템생명공학부 \*포항공과대 화학과

Amyloid  $\beta$  (A $\beta$ ) protein is known to cause Alzheimer's disease (AD), which is the most common neurodegenerative disease. A $\beta$  is produced by successive cleavage of amyloid precursor protein by  $\beta$ - and  $\gamma$ -secretase and consists of 39-43 amino acids because the cleavage sites of  $\gamma$ -secretase are various. Among A $\beta$ s with different size, A $\beta$ 1-42 is the major toxic species. Here we report hydrodynamic behavior of surface-conjugated A $\beta$ 1-42 observed by AFM force spectroscopy. A $\beta$ 1-42 was conjugated to the surface through its primary amine moieties, which locate at N-terminal and two lysines and recognized by anti-A $\beta$ 1-42 antibody, immobilized on AFM probe. By combining the dendron-surface chemistry and high-resolution AFM force-mapping, the characteristic behaviors of individual A $\beta$ s could be visualized. These results can be further used to study A $\beta$  distribution in fixed cell and tissue samples with high-resolution and sensitivity.

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발표분야: 분석화학

발표종류: 포스터, 발표일시: 금 15:00~17:00

## Recognition of the Nascent Polypeptide using AFM

이재은, 박준원

포항공과대 화학과

In plant cell, Arabidopsis ankyrin repeat protein (AKR2) can recognize the targeting signal of Arabidopsis chloroplast outer envelope membrane protein (OEP7) which is the nascent polypeptide and transport OEP7 to the chloroplast. AFM makes it possible to quantify directly the range and magnitude of the interaction forces between proteins. By using dendron-modified surface, sufficient lateral spacing can reduce steric hindrance, providing enhanced biomolecule detection. Here, we measured specific interaction forces between AKR2 and OEP7 with AFM to identify the recognition aspect. The quantitative analysis of protein-protein interaction can show the effect of transmembrane domain/C-terminal positive region (TMD/CPR)-type targeting signals of OEP7.

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발표종류: 포스터, 발표일시: 금 15:00~17:00

## Host-Guest Complexes Interaction Measured by Atomic Force Microscopy

배영인, 백강균, 김기문, 박준원

포항공과대 화학과

Atomic force microscopy (AFM) has been generally used to measure interactions of synthetic molecule pairs like host-guest complexes as well as biomolecule pairs. We measured the rupture forces of host-guest complexes, cucurbit[6]uril (CB[6]) and spermine. To observe rupture event of the complex at a single molecule level, the dendron was immobilized on both AFM tip and Si substrate. Then, dendron-modified tip was functionalized with the spermine. Especially, to measure specific rupture force on rigid surface, CB6 is immobilized on the dendron-modified substrate by using a bovine serum albumin (BSA). Under this condition, the specific force curves showing a nonlinear profile on the rigid surface were observed.

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발표종류: 포스터, 발표일시: 금 15:00~17:00

## Analysis of Copper plating solution using Capillary electrophoresis

장정우, 윤수영, 주재영, 권민혁, 임홍빈

단국대 화학과

Semiconductor manufacturing processes require various chemicals to plate Gold, Copper, and Nickel for wiring in the devices. Copper plating solution, one of the most important plating chemicals used in semiconductor manufacturing process has been mostly composed of Chloride, CuSO<sub>4</sub>, H<sub>2</sub>SO<sub>4</sub>, and some additives. At this point, the concentration of each chemical component is a main factor to control the process accurately for plating rate, plating level and shape. Monitoring of trace impurities is also required to control the process and recycle waste materials. However, existing analytical methods is too complicated and requires long analysis time. In this study, determination of the components in the etchant was carried out using capillary electrophoresis(CE). Since anions and cation can be determined by CE with small amount of sample and in a short time, some anions such as chloride, sulfate, and a cation, such as copper, in copper plating solution were separated simultaneously using capillary zone electrophoresis(CZE) with indirect detection mode. Tris, PDC, CTAB electrolytes and Chromate, Tris, PDC, CTAB electrolytes were used as buffers. The detection limits of each ingredient were determined in the range from 505 to 2317ug. The relative standard deviations (n=4) of the method were obtained between 0.38% and 10.25% for peak areas. Additionally, this optimized method was applied for the analysis of different types of Cu plating solutions used in the process.

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발표분야: 분석화학

발표종류: 포스터, 발표일시: 금 15:00~17:00

## **A synthesis of TiO<sub>2</sub> and SiO<sub>2</sub> nanoparticles for high dispersion**

김종민, 고정아, 안정원, 김수지, 임홍빈

단국대 화학과

Silica and Titania nanoparticles are widely used in various industrial fields for catalyst, cosmetic, paint, sensor, drug delivery, etc. Dispersion of those nanoparticles is primary of importance in solvents for industry. We produced size-controllable amorphous silica and titania nanoparticle via hydrolysis and condensation of Tetraethyl orthosilicate (TEOS) and titanium tetraisopropoxide (TTIP), respectively. The particle size was controlled by catalyst, stirring speed, reaction time and polymer binder at room temperature. And, dispersion of the particles was improved by surface modification or surfactant. The size of synthesized particles was determined by Field Emission Scanning Electron Microscope (FE-SEM), particle size analyzer and High-Resolution Transmission Electron Microscopy (HR-TEM). The dispersivity of the nanoparticles was also measured by a lab-built Turbidometry and compare with the other commercially available nanoparticles.



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발표코드: IV-ANAL.P-51

발표분야: 분석화학

발표종류: 포스터, 발표일시: 금 15:00~17:00

## Shotgun analysis of lipid extract from mouse brain by using comprehensive LC-MS<sup>E</sup>

박태성, \*배은정, \*김성환, 김영환

한국기초과학지원연구원 질량분석연구부 \*경북대 화학과

Lipidomics is a rapidly expanding research field in which multiple techniques are utilized to quantify the precise chemical constituents in a cell's lipidome and identify their cellular organization. The results obtained by lipidomics provide the information on their biochemical mechanisms through which lipids interact with each other and with crucial membrane-associated proteins. LC-MS has played an important role in the detection and identification of lipids. Especially, the ultra-performance liquid chromatography (UPLC) is now widely used and applied to not only lipid analysis and which have a high efficiency, resolving power, and sensitivity, and rapid analytic ability. In this study, a method for lipid profiling using UPLC coupled with mass spectrometry has been demonstrated for the analysis of mouse brain. For the analysis of lipids in biological samples, the use of MS<sup>E</sup> data results in multiple levels of information which is extremely useful when trying to confirm the identity of a specific compound. For the determination of the repeatability, linearity and recovery, the ratio of the peak areas of the endogenous lipid and the corresponding internal standard was calculated. On the other hand, MSE acquires all relevant information in both low energy and high energy acquisitions during the same analysis, and in the subsequent data processing available information on fragmentation pathways, diagnostic precursor and neutral losses allowed us to determine the polar head group and fatty acid composition in a relatively fast and efficient manner.

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발표코드: IV-ANAL.P-52

발표분야: 분석화학

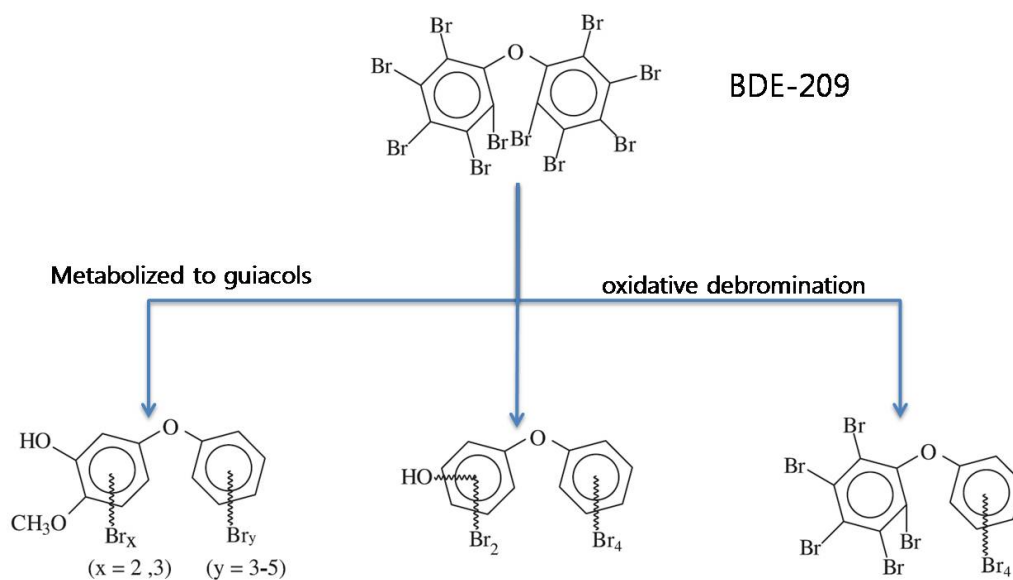
발표종류: 포스터, 발표일시: 금 15:00~17:00

## Metabolic profiling of rat exposed to decabromodiphenyl ether(DBDE)

서정주

한국기초과학지원연구원 서울센터

PBDEs may leach or volatilize from products and have been shown to bioaccumulate in the environment. Although bioaccumulation of PBDEs has been extensively studied several decades ago, little information is available about the metabolic characterization of PBDEs in animal models. In this work, we investigated the metabolic changes in rat forced-fed with decabromodiphenyl ether (DBDE) using NMR spectroscopy combined with multivariate statistical analysis. We obtained <sup>1</sup>H-NMR spectra of rat urine, plasma and liver tissue itself/extracts and identified some marker metabolites related with toxicity induced by DBDE using pattern recognition. This study provided the valuable information of metabolic difference between treatment and control group by using NMR-based metabolomics and could be applied for understanding the toxicity of DBDEs. In order to examine the bioavailability and bioaccumulation of PBDEs at low exposure levels, we have performed a mass balance study in rats fed a low dose of a Deca-BDE for 7 days. Suitable extraction and analytical methods were developed to achieve the chromatographic separation of decabromodiphenyl ether metabolites formed in vivo and to study their structure. This study provided the valuable information of metabolic difference between treatment and control group by using multivariate analysis and could be applied for understanding the toxicity of PBDEs.



Metabolites formed and identified by mass spectrometry following doses of BDE-209 in the rat.



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발표코드: IV-ANAL.P-53

발표분야: 분석화학

발표종류: 포스터, 발표일시: 금 15:00~17:00

## **In-house Preparation of Organic-inorganic Hybrid Monolith Column Bioreactor with Immobilized trypsin**

황효진, 오한빈

서강대 화학과

A simple type of immobilized trypsin bio-reactor based on organic-inorganic hybrid silica monolith has been prepared in a capillary column platform using a modified procedure of Ma et al [1]. A hybrid silica monolithic support was prepared using a traditional sol-gel method, in which tetraethoxysilane (TEOS) and 3-aminopropyltriethoxysilane (APTES) mixture were used as precursor materials. In addition, cetyltrimethyl ammonium bromide (CTAB) was used as a surfactant. In a synthesis procedure, pH control and amount of CTAB were found to be crucial. The performance of a trypsin-based micro-reactor was demonstrated by successfully digesting input of intact proteins into constituent pieces of peptides. The further details of the experimental results and procedure will be presented in the symposium.[1] J. Ma, Z. Liang, X. Qiao, Q. Deng, D. Tao, L. Zhang, Y. Zhang, Anal. Chem. 2008,80, 2949. This work is financially supported by Seoul R&D program(PA0910889)

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발표종류: 포스터, 발표일시: 금 15:00~17:00

## HPLC-UV를 이용한 식육 중 잔류Amprolium, Decoquinate 및 Dicyclanil의 분석

합현선, 공영진, 명승운

경기대 화학과

최근 동물용의약품은 가축의 질병 예방 및 치료, 성장 촉진을 위해 많은 농가에서 사용되고 있다. 동물용의약품이 가축의 생체내로 투여되어 축산물에 이행되고 잔류하게 되면 이를 섭취하는 사람들도 잔류하는 동물용의약품에 노출된다. 본 연구에서는 식육(소, 닭, 양) 중에 잔류하는 항콕시듬제(Amprolium, Decoquinate) 및 살충제(Dicyclanil)의 분석을 위한 시료 전처리방법 및 기기분석방법을 확립하였다. HLB (Hydrophilic-Lipophilic Balance) 카트리지를 사용한 고체상 추출법과 아세토나이트릴을 사용하여 시료를 효과적으로 추출 및 정제하였다. pH 5 로 조절된 메탄올과 물의 혼합물(1:1)을 HPLC 를 위한 reconstitution 용매로 사용하여 분석물의 동시분석을 행할 수 있었다. HPLC 의 효과적인 분리 및 분석을 위해 이동상으로는 이온쌍시약 20mM HFBA 와 메탄올 또는 메탄올과 아세토나이트릴의 혼합물(1:1.8)을 사용하였으며, 컬럼은 C18 (4.6mm × 250mm, 5μm)을 사용하였다. 확립된 전처리방법을 통해, 각각의 동물용의약품에 대한 검정곡선은 바탕시료에 분석물질의 0.051~12.0 mg/kg 의 농도로 소량첨가 시켜 분석한 결과 좋은 직선성( $r^2=0.997$  이상)을 보였으며, 11.5% 이하의 좋은 정밀도(RSD)를 보였다. 확립된 분석방법은 각각의 식육에 대한 항콕시듬제 및 살충제의 잔류허용기준(MRL, Maximum Residue Limits) 이하의 분석이 가능하였으며, 식육에 존재하여 amprolium 분석 시 방해물질로 작용하는 thiamine (Vitamine B1)과의 효과적인 분리를 실시하였다. 또한 통합 전처리방법을 통해 식육 중 동물용의약품의 모니터링이 가능하며 개별 전처리방법을 통해 동물용의약품의 정성 및 정량실험이 가능하였다.

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발표코드: IV-ANAL.P-55

발표분야: 분석화학

발표종류: 포스터, 발표일시: 금 15:00~17:00

## LC/ESI-MS/MS를 이용한 축산물(소, 돼지) 중 Phoxim 분석

이진주, \*명승운, \*조현우

경기대 자연과학부 화학과 \*경기대 화학과

축산물의 생산성 향상을 목적으로 한 과밀사육에서 질병예방 및 치료를 위해 항균성 물질을 포함한 동물성 의약품 중 하나인 Phoxim 은 돼지와 소, 양 등 축산물에 투여하는 구충제 및 살충제로 많이 사용되고 있다. 그러나 축산물 중으로의 이행, 잔류가 식품위생상 우려가 되고 있다. 본 연구에서는 LC/ESI-MS/MS 를 이용하여 돼지와 소 조직에서 Phoxim 을 분석하는 방법을 확립하였다. 먼저 균질화한 조직 시료를 아세트나이트릴로 추출하여 Silica 카트리지를 이용한 고체상 추출법으로 분석물질을 추출 및 정제할 수 있도록 하였고, 0.1% formic acid 를 포함하는 수용액과 아세트나이트릴을 이동상으로 사용하여 C18 컬럼(2.1×100 mm, 3.5  $\mu$ m; waters, U.S.A.)을 이용해 HPLC로 분리한 후 ESI-MS/MS 의 MRM 모드로 최적의 분석조건을 확립하였다. 돼지와 소에서의 회수율은 50.0%~70.0%, 검출한계와 정량한계는 각각 1.4~1.7 ng/kg 와 4.8~5.5 ng/kg 의 범위에서 나타났다. 검정곡선에서는 0.0048~2.0 mg/kg 의 농도범위에서 0.995 이상의 상관계수를 나타내었다. 확립된 분석방법은 정밀도, 정확도 및 회수율이 좋게 나타났으며 ng/kg 정도의 낮은 농도까지 분석하는 방법이었다

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발표코드: IV-ANAL.P-56

발표분야: 분석화학

발표종류: 포스터, 발표일시: 금 15:00~17:00

## LC/ESI-MS/MS 를 이용한 식육(소, 돼지, 닭), 우유 및 알에 잔류 하는 Monensin과 Salinomycin의 분석

마경나, \*명승운

경기대 자연과학부 화학과 \*경기대 화학과

monensin 과 salinomycin 은 소, 닭 등의 가축의 성장을 촉진시키고, 콕시듐증을 예방 및 치료하기 위해 사용되고 있다. 주로 사료를 통해 가축이 섭취하는 폴리에틸렌계 항생제인 두 물질은 식육, 우유, 알 등에 잔류하여 이것을 섭취하는 인간에게도 영향을 미칠 수 있다. 본 연구에서는 식육, 우유 및 알 중에 잔류하는 monensin 과 salinomycin 을 분석하기 위하여 Silica 카트리지를 이용하여 추출/정제하고 LC/ESI-MS/MS 를 사용하여 동시분석 하였다. 최적의 LC/MS 분석조건으로써 이동상은 각각 0.1%의 formic acid 가 포함된 아세트나이트릴과 수용액(94:6)으로 등용리용매조건에서 분석을 실시하였다. 컬럼은 C18 (2.1×100mm, 3.5μm), 유속 0.3 mL/min 의 조건에서 분리를 실시하였다. monensin 과 salinomycin 의 축산물에서 절대 회수율은 분석시료와 물질에 따라 차이를 보이지만 약 35-78% 의 범위에서 회수되었고, 검정곡선은 0.002-0.2 mg/kg 범위에서 상관계수(r<sup>2</sup>)가 0.99 이상으로 우수한 직선성을 나타냈다. 검출한계(LOD)는 0.0018-0.0036 mg/kg 로 나타났으며, 정량한계(LOQ)는 0.0017-0.0035 mg/kg 이었다. 분석의 정밀도를 측정한 결과 14.3 %(RSD) 이하를 보였다. 본 연구를 통하여 확립 된 분석법은 축산물에 잔류하는 monensin 과 salinomycin 의 잔류허용기준을 충분히 만족 할 수 있는 낮은 검출한계와 정량한계를 가지고 있으며, 동물용의약품의 정성 및 정량실험이 가능하였다.

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발표분야: 분석화학

발표종류: 포스터, 발표일시: 금 15:00~17:00

## Investigating the generation of the protonated ion by (+) mode APPI of polycyclic aromatic compounds: the role of toluene

AHMED ARIF, ISLAM ANANNA, 최철호, 김성환

경북대 화학과

Atmospheric pressure photo ionization (APPI) is a powerful technique for analysis of petroleum as well as polycyclic aromatic compounds. Analysis of polycyclic aromatic compounds is very important for environmental, drug and crude oil analyses. As a dopant or solvent, toluene is commonly used in APPI analysis. Toluene is especially important for the polycyclic aromatic compounds because they are soluble in toluene. Despite its importance, ionization mechanism of APPI using of toluene solvent was not thoroughly investigated. In this study, role of toluene molecules for the APPI process was investigated. Especially, mechanisms for the generation of molecular and protonated ions were studied. In the present study, temperature dependence experiments to study the mechanism of direct photoionization using different combination of solvents and samples were performed. Polyaromatic compounds such as naphthalene, anthracene, deuterated anthracene, acridine, pyrene, pentacene, benzoperylene, coronene and fullerene were used as samples and toluene, anisole, chlorobenzene, cyclohexane, hexane, acetonitrile and methanol were used as solvents. The APPI spectra demonstrate that the proton came from the toluene molecules and the hydrogen in methyl group of toluene molecules is used to produce protonated ion. Additionally, the direct connection between methyl group and aromatic ring is observed to be important for the protonation process. To study the ionization mechanism, ratio between molecular and protonated ions were monitored at various APPI source temperatures. A function relates ratio between abundance of molecular and protonated ions and APPI source temperature is a negative exponential function.



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발표분야: 분석화학

발표종류: 포스터, 발표일시: 금 15:00~17:00

## **A Quantitative Analysis for CIGS Thin Films by Dynamic Secondary Ion Mass Spectrometry**

임원철, \*이지혜, 원성욱, 이연희

KIST 특성분석센터 \*고려대 화학과

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 and the determination 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 very difficult to obtain by general analytical techniques. Dynamic SIMS has been widely used in an elemental analysis and a depth-profiling for a trace element existed on the surface because it is highly sensitive enough to detect small amount of ions at the level of ppm or ppb. There are various experimental conditions and factors to affect the SIMS depth profiling, such as primary ion, beam energy, beam current, raster size, surface roughness, position in the sample stage, and homogeneity of chemical composition of the sample, etc. Therefore, we evaluated Dynamic SIMS whether it is a suitable quantitative analysis technique for thin layer mixed with homogeneous bulk material such as CIGS. We have obtained a calibration curve to give the quantitative analysis information with low standard deviation.

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발표종류: 포스터, 발표일시: 금 15:00~17:00

## **Pd nanoparticles decorated carbon nanotube as an enhanced sensing platform for electrochemical detection of hydrogen peroxide**

정유나, 최현철

전남대 화학과

Accurate detection of H<sub>2</sub>O<sub>2</sub> rises from several practical reasons. Regarded to be a chemical threat agent, hydrogen peroxide spreads widely in rain and ground water as waste product of industry and atomic power stations. Because of its high oxidative property, it was used for disinfection of water pools, food and beverage packages. It is also the by-product of many enzymatic reactions and considered to be involved in progression of significant diseases. Therefore, accurate detection of H<sub>2</sub>O<sub>2</sub> is of crucial importance for environmental protection and healthy inspection. In this study, a simple method of depositing Pd nanoparticles onto carbon nanotubes (CNTs) as catalyst supports is devised for H<sub>2</sub>O<sub>2</sub> reduction. Amine groups were utilized as linkers to secure the Pd nanoparticles without agglomeration. The samples were characterized by TEM, XPS and Raman spectroscopy. The prepared CNT-Pd nanocomposites exhibit significant reduction of H<sub>2</sub>O<sub>2</sub>. This indicates that the Pd decorated CNTs have good electrocatalytic properties. Moreover, the electrode modified by the Pd-decorated CNTs exhibits a decrease in the overvoltage for H<sub>2</sub>O<sub>2</sub> reduction, which is favorable for low-potential amperometric detection.

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발표분야: 분석화학

발표종류: 포스터, 발표일시: 금 15:00~17:00

## **Preparation and Characterization of gold nanoparticle/graphene composites**

김지당, 최현철

전남대 화학과

The determination of hydrogen peroxide is of great importance in chemistry, biology, clinical control and environmental protection. Many techniques have been developed to detect hydrogen peroxide, including titrimetry, fluorimetry, spectrophotometry, chemiluminescence and electrochemical sensors. Among them, most involve high cost and are time consuming, except for electrochemical sensors. Due to their simplicity, high sensitivity and selectivity, electrochemical methods have been extensively employed in hydrogen peroxide determination. In this study, we have developed and characterized a biosensor for H<sub>2</sub>O<sub>2</sub> based on Au/graphene composites through glassy carbon electrode (GCE). The characterization of Au/graphene composites was performed with transmission electron microscopy (TEM), Raman and X-ray photoelectron Spectroscopy (XPS). Cyclic voltammetry (CV) and amperometric measurements were used to study and optimize the performance of H<sub>2</sub>O<sub>2</sub> biosensor.

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장소: 제주ICC

발표코드: IV-ANAL.P-61

발표분야: 분석화학

발표종류: 포스터, 발표일시: 금 15:00~17:00

## **Influence of thermal annealing on the microstructural properties of indium tin oxide nanoparticles**

김유현, 최현철

전남대 화학과

Since the electric conductivity of ITO nanoparticles is strongly dependent on the concentration of oxygen vacancies and the valence state of Sn, investigating the relationship between the microstructural changes and the preparation conditions is very important. Up to now, many researchers have studied the microstructural changes of ITO nanoparticles during the preparation process using various analysis tools. However, these reactions are very complicated and are not well understood. In this study, we investigated the microstructural changes of ITO during the annealing process. ITO nanoparticles were prepared by the sol-gel method using indium tin hydroxide as the precursor. To obtain detailed information about the microstructural changes of the ITO nanoparticles, we obtained their temperature-dependent in situ diffused reflectance infrared Fourier transform (DRIFT) spectra in the range of 80 - 360 oC. We also applied 2D correlation analysis to the DRIFT spectra in order to obtain the sequence of spectral events during the annealing process.

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발표분야: 분석화학

발표종류: 포스터, 발표일시: 금 15:00~17:00

## LC-MS analysis of fatty acids hydrolyzed from recombinant Escherichia coil

박선희

서강대 화학과

이 실험에서는 LC-MS 를 통하여 Escherichia coil 에서 추출한 fatty acids 을 분석하였다. 일반적으로 GC 를 이용한 fatty acid 분석은 liquid-liquid extraction and chemical derivatization steps 추출 단계를 거쳐 샘플준비에 많은 시간이 소모된다. 그러나 HPLC-MS 는 샘플 준비과정이 보다 간편하다. 추출한 혼합물을 가지고 LC-MS 를 통해 실험한 결과는 GC 를 이용한 실험 결과보다는 보다 더 sensitive 하다. Escherichia coil 에서 추출된 fatty acid 내에 qualitative analysis 을 통한 실험으로 Decanoic acid(C10:0), Myricstic acid(C14:0) Palmitic acid (C16:0), and Stearic acid (C18:0) 물질이 가장 많이 포함됨을 확인했다.

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장소: 제주ICC

발표코드: IV-ANAL.P-63

발표분야: 분석화학

발표종류: 포스터, 발표일시: 금 15:00~17:00

## Detection of hydrogen peroxide based on ruthenium complexes- modified carbon electrode

박초롱, 김혁한, 최영봉, 이금옥

단국대 화학과

Hydrogen peroxide ( $\text{H}_2\text{O}_2$ ) has been proven as a key reactive oxygen species in plant cells and its measurement in plant samples is very significant. Also,  $\text{H}_2\text{O}_2$  is a by-product of many biological oxidative reactions, e.g., glucose oxidase/glucose and other oxidases, therefore it is an very important parameter for monitoring biological processes. Extensive studies of hydrogen peroxide ( $\text{H}_2\text{O}_2$ ) have been done using horseradish peroxidase (HRP) that catalyzes hydrogen peroxide to water folloeing by two-electron reduction process. Although the enzymatic detection usually shows good selectivity and sensitivity, the activity of enzyme is easily decreased during its immobilization process. In this work we propose the detection of hydrogen peroxide with ruthenium complexes without horseradish peroxidase (HRP). Ruthenium complexes modified carbon electrode is presented for the electrochemical measurement of hydrogen peroxide at the physiological pH and at ambient temperature. These experimental facts showed that enzymeless  $\text{H}_2\text{O}_2$  sensor is one of a promising tools to develop a hydrogen peroxide sensor.

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발표분야: 분석화학

발표종류: 포스터, 발표일시: 금 15:00~17:00

## Synthesis and electrochemical characteristics of dopamine-tethered hippuric acid and Its application of immunoassay

이예림, 김혁한, 최영봉, 이정민

단국대 화학과

Urinary hippuric acid (HA), of molecular weight 180 Da, is one of the major metabolites in toluene-exposed humans and is a major biological indicator. Simple and ubiquitous monitoring of exposure to toluene is very important in occupational health care. We propose electrochemical immunoassay for rapid and quantitative detection of hippuric acid. The immunoassay system employs a conjugate of dopamine (DA) and hippuric acid (HA). As a electrochemical aspect, DA containing two hydroxyl group can show excellent redox signal. Also, dopamine-tethered hippuric acid (DA-HA) shows excellent redox signal in the immunoassay. The competition between HA and DA-HA generated electric signals proportional to HA concentration. The electrochemical immunoassay was comprised with DA-HA on the screen printed carbon electrode (SPCEs) and then apply the mixture antigen (HA) and HA-antibody. The electrical signal was measured by the voltammetry technique. The resulting currents were linearly related with the concentration of HA. Also the structures of DA-HA have been identified by the spectroscopic method and the electrochemical method.

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발표코드: IV-ANAL.P-65

발표분야: 분석화학

발표종류: 포스터, 발표일시: 금 15:00~17:00

## Coupling of headspace single drop microextraction with capillary electrophoresis

최정미, \*현재용, \*\*이동수, \*\*\*전형준, \*\*\*\*임종현, 정두수

서울대 화학부 \*서울과학기술대 2학년 8반 \*\*서울과학기술대 2학년재학 \*\*\*서울과학기술대 2학년 2반 \*\*\*\*  
서울과학기술대 2학년

Headspace single drop microextraction (HS-SDME) in-line coupled with capillary electrophoresis (CE) was performed to extract volatile analytes from an aqueous sample. Phenol and its derivatives as model acidic analytes of neutral forms in an aqueous donor solution were evaporated to the headspace above the solution and then back-extracted to a basic acceptor drop hanging at the tip of a capillary in a commercial CE instrument. The analytes in the acceptor of high pH became negatively charged and thus got enriched. The effects of the extraction time, salting-out, temperature, and agitation were investigated. The enrichment factors were about 200 times with 20-min extraction with agitation at 60°C. This proposed scheme was applied to tap water and proved to be a convenient sample preconcentration for CE analysis of volatile analytes in a real water sample.



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발표분야: 분석화학

발표종류: 포스터, 발표일시: 금 15:00~17:00

## Transient isotachophoresis of trace metals by on-capillary complexation in Zn(II) overloaded samples

박주령, 심은재, 최기환, 정두수

서울대 화학부

In capillary electrophoresis (CE) trace metal analysis combined with online preconcentration often receives interference from concentration disparity of the analytes in the sample. Here we demonstrate that saline samples overloaded with  $\text{Zn}^{2+}$  could be masked completely and selectively by adding thioglycolic acid (TGA) in the background electrolyte (BGE). It was observed that high concentrations of TGA (0.1 to 20 mM) in samples were unsuccessful to effectively mask  $\text{Zn}^{2+}$ . However, contrary to the usual procedure a complete masking could be achieved when Zn-overloaded samples devoid of TGA were analyzed using a BGE containing even a lower concentration (~0.5 mM) of TGA. A selective sweeping mechanism could be described as a means of masking in CE, which includes dynamic complexation and sweeping of  $\text{Zn}^{2+}$  selectively from the sample by TGA. While trace metals such as  $\text{Fe}^{2+}$ , and  $\text{Ni}^{2+}$  could be analyzed simultaneously by transient isotachophoresis (TITP) using 4-(2-pyridylazo) resorcinol (PAR) as a complexing agent. Chloride and PAR in the sample acted as the leading electrolyte and the terminating electrolyte, respectively. The optimized BGE was composed of 95 mM N-tris(hydroxymethyl)methyl-3-aminopropanesulfonic acid and 80 mM triethylamine, 0.1 mM PAR, 2 mM TGA and 0.02% FC-PN (a fluorocarbon neutral polymeric surfactant) at pH 9.0. The limits of detection ( $S/N = 3$ ) were in the sub ppb range ( $\text{Fe}^{2+}$  0.3 ppb,  $\text{Ni}^{2+}$  0.2 ppb). The method was successfully applied to determine the trace amounts of  $\text{Fe}^{2+}$  and  $\text{Ni}^{2+}$  in the standard reference urine and human urine samples containing excessive amounts of  $\text{Zn}^{2+}$ .

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발표코드: IV-ANAL.P-67

발표분야: 분석화학

발표종류: 포스터, 발표일시: 금 15:00~17:00

## Development of certified reference material for arsenobetaine analysis: preparation of arsenobetaine standard solution and certification by INAA and LC-ICP-MS

고경문, 김태규, \*이경석, \*임용현, \*임영란, \*황의진

부산대 화학과 \*한국표준과학연구원 분석화학표준센터

Arsenic (As) species are easily found in marine ecosystem and their toxicities are closely related to the chemical forms. Arsenic speciation analysis has been extensively studied to establish a public guideline for arsenic intake from sea foods. Arsenobetaine  $[(CH_3)_3AsCH_2COOH]$ , AsB is the most abundant arsenic species in sea foods such as fish and crustaceans, while it has very low toxicity compared with inorganic arsenic species. Therefore, accurate measurement of AsB is very important to evaluate effective toxicity due to arsenic species in sea foods. KRISS has developed AsB standard solution as a certified reference material (CRM) to provide reliability and traceability in AsB analysis. The AsB standard solution was prepared from highly pure AsB material. The total arsenic content in AsB standard solutions is measured by the instrumental neutron activation analysis (INAA) and the contribution of arsenic-containing impurities is determined by liquid chromatography coupled with inductively-coupled plasma mass spectrometry (LC-ICP/MS). Then, the certified value of arsenobetaine content is obtained by subtraction of the total amount of arsenic-containing impurities from the total content of arsenic. Liquid chromatography with C18 stationary phase and ion pairing reagents has been exploited to separate arsenic-containing impurities from the dominated AsB and, for method validation, ion exchange chromatography has been also used to insure complete separation. Preliminary homogeneity has been evaluated using 5 selected bottles. Complete characterization including homogeneity and stability will be carried out in the near future.

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장소: 제주ICC

발표코드: IV-ANAL.P-68

발표분야: 분석화학

발표종류: 포스터, 발표일시: 금 15:00~17:00

## **In-Line Coupling of Headspace-Single Drop Microextraction and Large Volume Stacking Using an Electroosmotic Flow Pump with a Commercial Capillary Electrophoresis Instrument**

박성태, 김지혜, 최기환, 정두수

서울대 화학부

Two sample preconcentration methods, headspace-single drop microextraction (HS-SDME) before injection and large volume stacking using an electroosmotic flow pump (LVSEP) after injection, were combined to improve the sensitivity of capillary electrophoresis (CE). By simple programming of liquid handling sequences of a commercial CE instrument, a basic aqueous drop was formed at the tip of a coated capillary, where a Teflon tube had been sleeved to serve as a hydrophobic support. When the drop was exposed over an acidic aqueous solution containing weakly acidic analytes, the analytes, exiting the matrix and passing the headspace of the donor solution in neutral forms, got enriched in the basic acceptor drop as negatively charged forms. Then the entire capillary column was filled with the enriched aqueous extract and LVSEP was carried out using a borate run buffer of high conductivity. The overall enrichment factors for the analytes 2-nitrophenol, 2,6-dichlorophenol, 2,3,6-trichlorophenol, and 2,4,6-trichlorophenol, from a combination of 30 min HS-SDME and LVSEP on a 60 cm capillary, were about 1000. No modification of the existing CE instrument was necessary and the difficulty of CE in handling highly saline matrices could be solved owing to the sample cleanup capability of SDME.

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장소: 제주ICC

발표코드: IV-ANAL.P-69

발표분야: 분석화학

발표종류: 포스터, 발표일시: 금 15:00~17:00

## Synthesis and electrochemical performance of multi-walled carbon nanotube/cyanobenzene functionalized polyaniline nanostructures

**M. Francklin Philips, \*A.Gopalan, \*\*이광필**

경북대 차세대에너지기술연구소 \*경북대 화학과 \*\*경북대 화학교육과

2-aminobenzonitrile (2-ABN) groups were incorporated into multiwall carbon nanotubes (MWNT) using graft copolymerization. A mixture of diphenylamine (DPA) and 2ABN was polymerized in the presence of MWNT. The resulting product, poly(diphenylamine-co-2-aminobenzonitrile)-grafted-MWNT (P(DPA-co-2ABN)-g-MWNT) was characterized by Raman spectroscopy, UV-Visible spectroscopy, X-ray diffraction analysis, Field emission- scanning electron microscope and atomic force microscope. The electrochemical characteristics of P(DPA-co-2ABN)-g-MWNT were evaluated by cyclic voltammetry. The incorporation of 2- ABN groups and presence of MWNT provide interesting properties to P(DPA-co-2ABN)-g-MWNT.

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장소: 제주ICC

발표코드: IV-ANAL.P-70

발표분야: 분석화학

발표종류: 포스터, 발표일시: 금 15:00~17:00

## Enantiomer Resolution of $\alpha$ -Amino Acid Esters as 9-Anthraldimine Derivatives Using Polysaccharide Derived Chiral Stationary Phases and Determination of Their Optical Purity

이원재, 황호, 서문준

조선대 약학대학

The chromatographic enantiomer resolution of  $\alpha$ -amino acid methyl and ethyl esters as 9-anthraldimine derivatives on polysaccharide-derived chiral stationary phases (CSPs) was performed. The 9-anthraldehyde Schiff base derivatives of  $\alpha$ -amino acid esters were readily synthesized by stirring the  $\alpha$ -amino acid ester hydrochloride salts with 9-anthraldehyde in the presence of a base and anhydrous  $\text{MgSO}_4$ . Among all examined CSPs, Chiralcel OD or Chiralcel OD-H showed the greatest enantiomer resolution of 9-anthraldimine derivatives of  $\alpha$ -amino acid methyl and ethyl esters. It was notable that the L-enantiomers of all the analytes were preferentially retained on Chiralcel OD or Chiralcel OD-H. This developed analytical method was applied to determine optical purities of several commercially available D- or L- $\alpha$ -amino acid methyl esters.

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장소: 제주ICC

발표코드: IV-ANAL.P-71

발표분야: 분석화학

발표종류: 포스터, 발표일시: 금 15:00~17:00

## One-pot synthesis of copper nanoparticles loaded conducting polymer composites

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Poly(4-aminodiphenylamine)-copper nanocomposites (P4ADPA/CuNC) were prepared by the facile one step aqueous chemical oxidative dispersion polymerization of 4-aminodiphenylamine (4ADPA) using copper sulfate as an oxidant in p-toluene sulfonic acid medium. 4ADPA was oxidized by CuSO<sub>4</sub>, yielding P4ADPA and elemental Cu simultaneously. The P4ADPA/CuNC was characterized by Field emission-scanning electron microscope, X-ray diffraction analysis, Fourier transformer infrared spectroscopy, thermogravimetric analysis and UV-Visible spectroscopy.

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장소: 제주ICC

발표코드: IV-ANAL.P-72

발표분야: 분석화학

발표종류: 포스터, 발표일시: 금 15:00~17:00

## Preparation and characterization of nanodiamond-conducting polymer nanomeshes

A.Gopalan, Shanmuga sundaram Komathi, \*이광필

경북대 화학과 \*경북대 화학교육과

Bulk quantity of three dimensional (3D) nanodiamond (ND)-conducting polymer nanomeshes was prepared by chemical oxidative polymerization. ND was amine functionalized (ND-NH<sub>2</sub>) and subsequently linked to conducting polymer 3D networks ((designated as ND-PANI-3DNW) through cross-linking assisted polymerization. The morphology of the ND based nanomeshes was examined by field emission scanning electron microscopy. Structural aspects and electronic properties of ND-PANI-3DNW were investigated by Fourier transform infrared spectroscopy, X-ray diffraction measurements and UV-visible spectroscopy. The effectiveness of ND-PANI-3D(NW) was evaluated towards removal of hexavalent Cr ion (Cr(VI)) from industrial/drinking water.

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발표분야: 분석화학

발표종류: 포스터, 발표일시: 금 15:00~17:00

## 스크린 프린팅 방법을 기반으로 한 평면형 타입의 소형 산소 센서

김민수, 김현숙, 문태일, 강태영

(주)아이센스 부설연구소

혈액 내 산소 농도의 측정은 임상학적으로 매우 중요한 부분을 차지하고 있으며 보다 쉽고 정확하게 그리고 경제적으로 검출하기 위한 소형 화학센서의 개발이 활발히 진행되고 있다. 본 연구에 사용된 산소 센서는 스크린 프린팅 방법을 바탕으로 여러 개의 전기화학 센서(electrochemical sensor)와 함께 평면형 소형 센서 위에 제작하였다. 스크린 프린팅 방법의 사용은 제조 시 마다 모든 전극이 균일하게 형성되므로 센서의 성능을 일정하게 유지시킬 수 있으며 대량생산에 용이하다는 장점을 가진다. 산소 센서는 전기화학적 방법을 이용한 3-전극계 전류법(amperometry) 산소 전극을 사용하였으며, 전류법 산소 전극은 작동 전극(working electrode)에서 발생하는 산소 환원 전류로부터 산소량을 측정하는 방법으로 작동 전극의 소형화가 매우 중요하다. 본 연구에서는 직경 50  $\mu\text{m}$ 의 원형 작동 전극을 스크린 프린팅 방법으로 구현하였고, Gas permeable polymeric membrane 을 사용하여 산소 센서를 제작하였다. 이와 같이 제작된 산소 센서는 2 주 이상의 우수한 감응성, 직선성 및 재현성을 유지하였다. 또한 상용화된 타사의 분석기(Radiometer 사 ABL835)와 혈액시료에 대한 측정값을 비교해 본 결과 매우 유사한 성능을 나타냈다.



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발표코드: IV-ANAL.P-74

발표분야: 분석화학

발표종류: 포스터, 발표일시: 금 15:00~17:00

## **Preparation and properties of two dimensional carbon nanostructure dispersed conducting polymers**

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경북대 화학교육과 \*Rajalakshmi Engineering college, Thandalam, Chennai, India

Conducting polymers have been shown as promising materials because of their high conductivity and fast redox activity. Generally, carbon nanomaterials are dispersed in conducting polymer matrixes to form for flexible electronics, electromagnetic shielding, and energy storage device applications. These conducting polymer/ carbon nanostructures possess both the properties of conducting polymer and carbon nanostructures. A new two dimensional carbon nanostructure dispersed conducting polymer composite (CPCNS) has been prepared by simple one step oxidative polymerization. The morphology and microstructure of the resultant CPCNS are characterized by field emission scanning electron microscopy (FESEM), Thermogravimetric analysis (TGA) and Raman spectroscopy. The optical properties of CPCNS were investigated by UV-visible absorption and photoluminescence spectroscopies. The electrochemical behavior and the band-gap of CPCNS were evaluated by cyclic voltammetry and UV-vis spectroscopy.

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발표코드: IV-ANAL.P-75

발표분야: 분석화학

발표종류: 포스터, 발표일시: 금 15:00~17:00

## Preparation and characterization of cobalt-palladium bimetallic particles distributed carbon nanotubes by gamma irradiation

이세희, \*Shanmuga sundaram Komathi, \*A.Gopalan, \*\*이광필

경북대 나노과학기술학과 \*경북대 화학과 \*\*경북대 화학교육과

Thiol functionalized multiwalled carbon nanotubes (MWNT-T) were dispersed with cobalt-palladium bimetallic particles (MWNT-T/Co-Pd NPs) by gamma irradiation method.. MWNT-T/Co-Pd NPs composites were characterized by field emission scanning microscopy, UV-visible spectroscopy, X-ray diffraction analysis, thermogravimetric analysis and Raman spectroscopy. The effects of composition of Pd to Co, stabilizing effect of thiol groups and irradiation dosage levels on the distribution of catalyst particles were analyzed. The electrocatalytic activities of MWNT-T/Co-Pd NPs catalyst modified electrodes were investigated by cyclic voltammetry.

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장소: 제주ICC

발표코드: IV-ANAL.P-76

발표분야: 분석화학

발표종류: 포스터, 발표일시: 금 15:00~17:00

## Synthesis, characterization novel polymer composite membranes based on sulfonated poly(ether ether ketone) for fuel cell application

이세희, \*M. Francklin Philips, \*\*A.Gopalan, \*\*\*이광필

경북대 나노과학기술과 \*경북대 차세대에너지기술연구소 \*\*경북대 화학과 \*\*\*경북대 화학교육과

Sulfonated polyether ether ketone (SPEEK) is prepd. by the sulfonation of polyether ether ketone (PEEK). New hybrid organic-Inorganic composite membrane based on sulfonated poly(ether ether ketone) (SPEEK) silica (SiO<sub>2</sub>) were subsequently prepared for various conditions such as percentage compositions of the SPEEK, and silica.. The prepd. composite membranes were characterized using Fourier transform IR spectroscopy, x-ray diffraction and thermogravimetric analysis.. Surface morphology of the composite membranes was analyzed using scanning electron microscopy. Other properties related to conductivities (ion exchange capacity, (IEC), proton cond.), absorptivity (water and methanol absorption) and durability were also evaluated for the composite membranes.. These composites also showed good conductivities, and durabilities. Hence, these composite membranes have the potential to be used in the development of newer proton exchange membrane fuel cells.

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발표코드: IV-ANAL.P-77

발표분야: 분석화학

발표종류: 포스터, 발표일시: 금 15:00~17:00

## Facile synthesis of new multi-functional iron oxide-gold nanocomposites using $\gamma$ -radiation

김민경, A.Gopalan, \*이광필

경북대 화학과 \*경북대 화학교육과

We report a facile approach for the preparation of new multi-functional iron oxide-gold nanostructure composites using  $\gamma$ -radiation. Initially, iron oxide nanoparticles were prepared by co-precipitation method and then functionalized with thiol groups. The thiol functionalized iron oxide nanoparticles were coated with gold nanostructures using  $\gamma$ -radiation induced reduction in the presence of a functional surfactant. UV-visible spectroscopy, scanning electron microscopy, X-ray diffraction analysis and magnetic measurements were used to characterize the new iron oxide-gold nanocomposites. The new nanocomposites are expected to find application in optical/magnetic resonance bimodal imaging, opto-magnetic therapy, catalysis and magnetic separation.

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발표코드: IV-ANAL.P-78

발표분야: 분석화학

발표종류: 포스터, 발표일시: 금 15:00~17:00

## Simultaneous quantitation of Dopa, L-dopa, L- $\alpha$ -dopa, 3-O-Methyldopa, Benserazide and Entacapone in rat plasma by LC-ESI-MS/MS

박세민, 최용근, 이지은, 하세영, 이정한

경상대 화학과

Highly sensitive, selective and rapid assay method by high-performance liquid chromatography-tandem mass spectrometry (LC-MS/MS) was developed for dopa, L-dopa, L- $\alpha$ -dopa, 3-O-methyldopa, benserazide and entacapone in rat plasma and applied to a pharmacokinetic study. Sample pretreatment and clean-up were performed by a liquid-liquid extraction. Carbidopa 1000 ng/mL was used as an internal standard. Run time was 10 min and good linearity was achieved between 50 and 1,000 ng/mL for the analytes. The analytes were separated by a Zorbax XDB C<sub>18</sub> column with the mobile phase composed of methanol and 0.5% aqueous formic acid (50:50, v/v) and monitored in MRM mode

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발표코드: IV-ANAL.P-79

발표분야: 분석화학

발표종류: 포스터, 발표일시: 금 15:00~17:00

## Determination of flavonoid components as defense materials of onion against *Fusarium* sp. using liquid chromatography coupled with tandem mass spectrometry

최용근, \*정성우, 이정한, 박세민, 서온누리, 이지은, 하세영, 신성철

경상대 화학과 \*경상대 원예학과

Basal rot caused by *Fusarium* sp. is one of the most important diseases in pre- and postharvest of onion. A total of eleven flavonoid components (quercetin 3,7,4'-triglucoside, Quercetin dihexoside, quercetin 7,4'-diglucoside, quercetin 3,4'-diglucoside, quercetin 3-glucoside isorhamnetin 4'-galactoside, Isorhamnetin 3,4'-diglucoside, quercetin 4'-glucoside, isorhamnetin 4'-glucoside, Quercetin, Isorhamnetin) were characterized for the onion bulb infected by *Fusarium* sp. In order to obtain an insight into the flavonoids as the defense materials of the onion, the onion bulb was inoculated by the fungus and the content change of flavanoids was monitored by HPLC over eight day post-infection.

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발표코드: IV-ANAL.P-80

발표분야: 분석화학

발표종류: 포스터, 발표일시: 금 15:00~17:00

## **Analysis of polyphenols in soybean sprout infected by *Colletotrichum gloeosporioides* using LC-MS/MS**

이정환, 박세민, 최용근, 이지은, 하세영

경상대 화학과

Soybean sprout is an important nutrient vegetable. One of the most serious diseases of soybean sprout culture is anthracnose induced by *Colletotrichum gloeosporioides*. The disease causes hypocotyls black spots and cotyledon black lesions on soybean sprout. The objective of this study was to the analysis of polyphenols as defense secondary metabolites in soybean (*Glycine max* (L.) Merrill) sprouts infected by *Colletotrichum gloeosporioides*. One amino acid and twelve flavonoids were identified and quantified by LC-MS/MS.

일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: IV-ANAL.P-81

발표분야: 분석화학

발표종류: 포스터, 발표일시: 금 15:00~17:00

## Characterization of polyphenols in *Lonicera japonica* Thunb. using HPLC-MS/MS

서은누리, 박세민, 이정한, 신성철

경상대 화학과

The *Lonicera japonica* Thunb. Has been commonly used in traditional Chinese medicine for the treatment of various diseases, including arthritis, diabetes mellitus, antidote, to treat urinary disorders, headache, fever, infections, sores, swelling and so on. The *L. japonica* Thunb. was analyzed for polyphenols via high performance liquid chromatography coupled with tandem mass spectrometry (HPLC-MS/MS) in the positive mode and negative with selected ion monitoring.



일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: IV-ANAL.P-82

발표분야: 분석화학

발표종류: 포스터, 발표일시: 금 15:00~17:00

## Background Level Concentrations of Atmospheric Radon ( $^{222}\text{Rn}$ ) Measured at Gosan Site of Jeju Island, Korea during 2008-2009

고희정, 신승희, 강창희, 김원형, 변종철

제주대 화학과

The real-time radon( $^{222}\text{Rn}$ ) concentration measurement has been carried out in order to evaluate the background level concentrations of atmospheric radon in Gosan site, Jeju Island, for two years between January 2008 and December 2009. The  $^{222}\text{Rn}$  concentration at Gosan was  $2,702 \pm 1,286$  mBq/m<sup>3</sup> during the study period, and its seasonal concentrations were 2,564, 2,044, 3,086 and 3,128 mBq/m<sup>3</sup> respectively for spring, summer, fall and winter seasons. The monthly radon concentrations were in the order of Feb > Sep > Oct > Dec > Nov > Jan > Mar > Apr > Aug > May > Jun > Jul, and the concentration in February was 2.1 times higher than that in July. From the comparison of hourly concentrations, it has increased during the nighttime with the highest concentration at 7 a.m., and relatively decreased during the daytime with the lowest value at 3 p.m. Based on the back trajectory analysis, the radon concentrations showed high values when the air mass moved from the China continent to Jeju area, on the other hand, they showed low values when moving from the North Pacific Ocean.

일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: IV-ANAL.P-83

발표분야: 분석화학

발표종류: 포스터, 발표일시: 금 15:00~17:00

## Chemical Composition of Size-segregated Atmospheric Aerosols at Jeju Island, Korea during Asian Dust Event in 2010

이순봉, 고희정, 강창희, 김원형, 김덕수

제주대 화학과

The size-segregated atmospheric aerosols have been collected at Jeju island, Korea in spring time of 2010, and analyzed in order to investigate the characteristics as well as their composition changes during Asian Dust and Non-Asian Dust events. During the heaviest Asian Dust event on March 20 ~ 21, the  $\text{nss-Ca}^{2+}$  concentration in TSP (total suspended particles) was  $7.72 \mu\text{g}/\text{m}^3$  which was 10.8 times higher compared to those during Non-Asian Dust periods. And the concentrations of  $\text{nss-Ca}^{2+}$ ,  $\text{NO}_3^-$ , Al, Ca, Fe in  $\text{PM}_{10}$  aerosols were 11.08, 8.68, 11.91, 4.42,  $9.89 \mu\text{g}/\text{m}^3$ , which were 17.5, 1.8, 9.3, 8.6, 8.6 times higher during Asian Dust event, respectively. Furthermore, the concentrations of  $\text{nss-Ca}^{2+}$ ,  $\text{nss-SO}_4^{2-}$ ,  $\text{NO}_3^-$  in  $\text{PM}_{2.5}$  aerosols increased up to 1.11, 7.47,  $4.70 \mu\text{g}/\text{m}^3$ , showing 16.3, 1.1, 2.1 times higher, respectively. From the comparison of size-segregated aerosol compositions, the concentration ratios of anthropogenic  $\text{nss-SO}_4^{2-}$ ,  $\text{NO}_3^-$ , and S between Asian Dust and Non-Asian Dust events were 1.0, 2.7, 1.4 in fine particles, and 8.4, 2.9, 13.3 in coarse particles, respectively. Meanwhile, those of soil originated  $\text{nss-Ca}^{2+}$ , Al, Ca, Fe were 5.3, 3.8, 12.4, 14.2 in fine particles, and 49.0, 15.2, 10.2, 15.0 in coarse particles, respectively.

일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: IV-ANAL.P-84

발표분야: 분석화학

발표종류: 포스터, 발표일시: 금 15:00~17:00

## **Rapid and sensitive determination of Nebivolol in human plasma by liquid chromatography-electrospray ionization tandem mass spectrometry**

김수지, 장해종

ISS ART

Nebivolol was determined in human plasma by HPLC-MS/MS using nebivolol-d4 as an internal standard. To simplification of extraction steps and optimization of chromatographic condition, sample preparation method was accomplished using protein precipitation. The mobile phase was composed of 40 % acetonitrile and 60% 1 mM Ammonium Formate (with 0.1% formic acid) and total run time was 2.2 min. The LC-MS/MS system was equipped with an electrospray source operating in the positive ion mode. The limit of quantification (LOQ) was 25 pg/mL, using a sample volume of 400  $\mu$ L for the analysis. The reproducibility of the method was evaluated by analyzing five replicates at four quality control (QC) levels over the nominal concentration range 25 to 5000 pg/mL. Nebivolol produced a protonated precursor ion ( $[M+H]^+$ ) at  $m/z$  406, and a corresponding product ion at  $m/z$  151. Internal standard produced a protonated precursor ion ( $[M+H]^+$ ) at  $m/z$  410 and a corresponding product ion at  $m/z$  151. The validation, reproducibility, stability, and recovery of the method were evaluated. The method has been successfully applied to pharmacokinetic studies of nebivolol in human plasma.

일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: IV-ANAL.P-85

발표분야: 분석화학

발표종류: 포스터, 발표일시: 금 15:00~17:00

## **Resolution of Proton Pump Inhibitors on two Ligand Exchange Chiral Stationary Phases based on (S)-Leucinol**

한혜지, 현명호

부산대 화학과

We wish to report the enantioselective separation of racemic proton pump inhibitors (PPIs) including omeprazole on two ligand exchange CSPs. One is based on (S)-leucinol derivative, sodium N-((S)-1-hydroxymethyl-3-methylbutyl)-N-undecylaminoacetate covalently bonded to silica gel. Another is a CSP prepared by introducing n-octyl groups onto the residual silanol groups of the first CSP. These two ligand exchange CSPs were successfully applied to the resolution of PPIs. The CSP containing residual silanol-protecting n-octyl group was found to be better than the original CSP in the resolution of PPIs.

일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: IV-ANAL.P-86

발표분야: 분석화학

발표종류: 포스터, 발표일시: 금 15:00~17:00

## Host-Guest Chemistry in Gas Phase: Unusual Stability of $\alpha$ -helix Conformation of 18-Crown-6 Complex of Alanine Based Polypeptide

고재훈, 허성우, 김승빈, 김준곤

포항공과대 화학과

The gas phase conformations of alanine based polypeptides are studied with different locations of a lysine residue and host-guest interactions with 18-crown-6 ether (18C6). Gas phase conformation of a series of model peptides  $(\text{Ala})_m\text{Lys}(\text{Ala})_n$ , where  $m + n = 9$ , is examined alone and with 18C6 using traveling ion mobility mass spectrometry. Doubly charged peptide ions are generated in the gas phase using electrospray ionization methodology. We find that self solvation plays a major role in forming the secondary structure of a peptide in the gas phase. We observe the propensity of alanine based peptides to form  $\alpha$ -helices in the gas phase when Lys residue is located close to C-terminus so the interaction between Lys and C-terminal carboxyl group exert its effect negligibly on the secondary structure. In the case of peptides, which a Lys residue is close to N-terminus, globular conformation is observed exclusively. Blocking Lys residue using 18C6 yields changes in gas phase peptide conformations of all model peptides investigated in this study. Molecular dynamics simulations of 18C6 complexes of model peptides correlate well with experimental observations and provide a detailed picture of the interactions between the Lys residue, C-terminal carboxyl group, N-terminal ammonium group, and 18C6 in the gas phase.

일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: IV-ANAL.P-87

발표분야: 분석화학

발표종류: 포스터, 발표일시: 금 15:00~17:00

## Extractive ethoxycarbonylation for enhanced detectability of 19 urinary estrogens down to pg/mL levels in GC-MS based analysis

문주연, \*문명희, \*\*정봉철, \*\*최만호

연세대 화학과/KIST \*연세대 화학과 \*\*KIST 생명보건본부

Endogenous estrogens, including catechol estrogens (2- or 4-hydroxy-estrone and 17 $\beta$ -estradiol) play an important role in the development of female-related disorders and the homeostasis of bone. To overcome their high polarity and instability in gas chromatography-mass spectrometry (GC-MS) based analysis, a comprehensive technique was conducted with the two-phase extractive ethoxycarbonylation (EOC) of the phenolic hydroxy groups of estrogen with ethyl chloroformate on n-hexane extraction, which could diminish the matrix interference. And the subsequent pentafluoropropionylation (PFP) of the remaining aliphatic hydroxyl groups of estrogens was introduced. The sample was separated through a high temperature GC column (MXT-1) within an 8-min running and detected in the selected-ion monitoring mode. The analytical conditions led to well separated with a good peak shape for 19 estrogens as their EOC-PFP derivatives. The limit of quantification (LOQ) were 0.02 ~ 0.1 ng/mL for most estrogens analyzed except for 2-hydroxyestriol (0.5 ng/mL). The devised method was found to be linear (correlation coefficient,  $r^2$  = 0.995) in the range from LOQ to 40 ng/mL, while precisions (% CV) and accuracies (% bias) ranged from 1.4% to 10.5% and 91.4 to 108.5%, respectively. To demonstrate the usefulness of this novel method, the urinary levels obtained from 100 postmenopausal female patients with osteoporosis were measured due to their low urinary concentrations. The present technique can be a useful for clinical diagnosis as well as understanding pathogenesis in estrogen-related disorders.

일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: IV-ANAL.P-88

발표분야: 분석화학

발표종류: 포스터, 발표일시: 금 15:00~17:00

## **Steroid signatures in serum and urine reveal the different metabolic pathways between precocious puberty girls**

강세미, \*문주연, \*\*최만호, 홍종기, \*\*정봉철

경희대 약학과 \*연세대 화학과 \*\*KIST 생명보건본부

Precocious puberty (PP) is responsible for either central activation of the hypothalamic-pituitary-gonadal (HPG) axis (true-PP) or to an abnormal steroid production that does not result from sustained activation of the HPG axis (peripheral-PP). The gas chromatography-mass spectrometry based steroid assay in both serum and urine was applied to patients with both 43 true-PPs and 41 peripheral-PPs to evaluate altered metabolic patterns against 33 age-matched healthy girls. Although not exactly the same patterns of steroid metabolism between serum and urine samples, the levels of testosterone were tended to increase in both PP patients ( $P < 0.02$ ), especially in true-PP ( $P < 0.005$ ). In serum, androstenedione and 11-dehydrocorticosterone could differentiate true-PP from peripheral-PP ( $P < 0.003$  and  $0.0003$ , respectively). In urine, the levels of estrone were increased in true-PP compared to peripheral-PP ( $P < 0.01$ ), and epitestosterone,  $16\alpha$ -OH-DHEA,  $17\beta$ -estradiol and estriol were significantly increased in only true-PP ( $P < 0.005$ ). The activity of  $11\beta$ -HSD1 was decreased in both PP patients ( $P < 0.01$ ), while  $11\beta$ -HSD2 and aromatase were remarkably up-regulated in serum samples obtained from both patient groups ( $P < 0.005$ ). The results could be explained that the level of testosterone activated by luteinizing hormone is decreased in peripheral-PPs when most estrogens and two active androgens, epitestosterone and  $16\alpha$ -OH-DHEA, are up-regulated in both PP groups.

일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: IV-ANAL.P-89

발표분야: 분석화학

발표종류: 포스터, 발표일시: 금 15:00~17:00

## **Analysis of polyphenolic compounds in red bell pepper infected by anthracnose using LC-MS/MS**

하세영, 이지은, 최용근, 이정환, 신성철, 서은누리, 박세민, \*정성우

경상대 화학과 \*경상대 원예학과

Anthrachnose, caused by *Colletotrichum* sp., attacks a wide variety of vegetables, legumes, and fruit crops. Especially, anthracnose is a very frequent disease of solanaceous crops. In this study, polyphenolic compounds in red bell pepper infected by *Colletotrichum* sp. were determined and the content change of polyphenolic compounds was monitored by HPLC over 144 hr post-infection.



일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: IV-ANAL.P-90

발표분야: 분석화학

발표종류: 포스터, 발표일시: 금 15:00~17:00

## Enhanced Raman scattering with nanoparticle-terminated tip

박찬규, 김주영, 김지환

고려대 화학과

We report on the implementation of metallic (Ag or Au) nanoparticle (NP)-terminated tip for the tip-enhanced Raman scattering (TERS). The NP-tip is fabricated by the mechanical pickup of individual NPs onto the surface of silicon tip that is pre-functionalized with 3-aminopropyltrimethoxysilane layers. We find that the metallic junction formed by the NP-tip - organic monolayer- Au thin film provides at least one order of magnitude larger Raman signals than the ones from a more conventional TERS junction (metallized tip - organic monolayer - Au film), which is reproduced by the classical electrodynamics simulation.

일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: IV-ANAL.P-91

발표분야: 분석화학

발표종류: 포스터, 발표일시: 금 15:00~17:00

## 수용액 매질 내 우라늄 농도 정량분석

### 정의창, 조혜륜

한국원자력연구원 원자력화학연구부

수용액 매질에 존재하는 우라늄의 정량분석 방법으로 분광광도계를 이용하는 흡수 분광법, 형광광도계를 이용하는 형광 분광법 등을 꼽을 수 있다. 특히, 펄스 레이저를 광원으로 이용하는 형광 분광법은 측정 감도가 우수하므로 ppb (parts per billion) 이하의 극미량 농도 분석이 가능하다. 현재까지 알려진 이러한 방법은 농도를 알고 있는 표준 시료를 이용해 검정 곡선(calibration curve)을 구한 후, 이 곡선에 미지 시료에서 측정된 신호를 대입하여 정량분석을 하고 있다. 이러한 경우, 광원의 세기, 검출기의 감도 등에 따라 검정 곡선의 기울기가 달라질 수 있으므로 미지 시료를 측정할 때 마다 검정 곡선을 새로 구해야 한다. 이 연구에서는 수용액 매질에 포함된 우라늄의 경우, 물의 라만산란 세기와 우라늄 형광 세기의 비를 이용하는 새로운 우라늄 정량분석 방법을 개발하였다. 광원 세기와 검출기 감도 등의 측정 조건이 변할 때 검정 곡선을 반복적으로 측정해야 하는 기존 방법의 번거로움을 줄일 수 있었다. 이 방법으로 구한 우라늄 정량분석의 검출한계를 제시한다.

일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: IV-ANAL.P-92

발표분야: 분석화학

발표종류: 포스터, 발표일시: 금 15:00~17:00

## A study about properties of synthesized Ti-hydrotalcite as a highly efficient plastic additives

김지혜, 김종원, 정용석, 권수한

충북대 화학과

하이드로탈사이트는 음이온 포획능력이 뛰어나고 내열성이 강한 특성이 있어서 고분자의 첨가제로 많이 사용되고 있다. 본 연구는 첨가제로서 사용되는 하이드로탈사이트를 전기분해법을 이용하여 티타늄을 표면에 침착시킨 Ti-하이드로탈사이트로 합성하여, 기존의 하이드로탈사이트보다 Ti-하이드로탈사이트를 첨가제로 사용하였을 때에 첨가제로서 고효율적인 성질이 나타나는지 여러 가지 방법으로 알아본다. 본 연구는 교육과학기술부와 한국산업기술재단의 지역혁신인력양성사업으로 수행된 연구결과임.

일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: IV-ANAL.P-93

발표분야: 분석화학

발표종류: 포스터, 발표일시: 금 15:00~17:00

## 시간분해 레이저 형광 분광학을 이용한 극미량 우라늄 화학종 규명

조혜륜, 정의창, 박경균, 차완식, 송규석

한국원자력연구원 원자력화학연구부

방사성 폐기물의 처분 안전성을 예측하기 위해 지하수 매질에 극미량으로 존재하는 악티나이드 화학종 규명 (chemical speciation) 연구가 필요하다. 이를 위한 효과적인 방법으로 레이저 분광기술을 꼽을 수 있다. 특히 시간분해 레이저 형광 분광학 (TRLFS, Time-Resolved Laser Fluorescence Spectroscopy) 기술은 특정 대상 원소에 대해 선택성이 높은 고감도 분광기술로 극미량 우라늄 화학종의 정성 및 정량분석에 효과적이다. 지하수에 포함된 우라늄은 일반적으로 물 분자와 반응하여 우라늄 가수분해 화학종(U(VI)-OH)을 형성한다. 또한 지하수에 존재하는 미량의 유/무기 리간드와 반응하여 용존 복합체를 형성하거나 지하수가 접촉하고 있는 광물표면에 흡착됨으로써 새로운 표면 복합체를 형성한다. 과량의 탄산이온을 포함하고 있는 지표수에 포함된 우라늄의 경우에는 안정한 상태의 U(VI)-CO<sub>3</sub> 화학종을 형성하기도 한다. 이 연구에서는 TRLFS 기술을 이용하여 자연계에 안정하게 존재하는 대표적인 우라늄 화학종인 U(VI)-OH 및 U(VI)-CO<sub>3</sub> 복합체의 형광 스펙트럼을 조사하였다. 488, 509, 533, 559 nm 파장의 특징적인 형광 봉우리를 나타내는 UO<sub>2</sub><sup>2+</sup> 이온의 형광 특성이 가수분해 화학종의 형성에 따라 장파장 방향으로 이동하고, 탄산이온 착물 형성에 따라 단파장 방향으로 이동하는 양상을 관측하였다. 또한 자연계 광물의 대표적인 성분인 실리카 표면에 흡착된 U(VI) 화학종의 형광 특성과 U(VI)-SiO<sub>2</sub> 흡착 거동이 또 다른 금속이온의 화학적 거동에 미치는 영향을 보고한다.

일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: IV-ANAL.P-94

발표분야: 분석화학

발표종류: 포스터, 발표일시: 금 15:00~17:00

## **A selective chemometric fluoride sensor based on the derivative with urea groups**

이은빈, 김관겸, 김동완, 김재상

경상대 화학과

A new colorimetric sensors containing urea(1) and thiourea(2) moieties for fluoride were designed and synthesized. These simple receptors were characterized their stoichiometry, and investigates the mechanism of their selectivity as anion receptors. The addition of tetrabutylammonium fluoride salts to the solution of receptors caused a dramatically and clearly observable color changes from light to yellow or red, respectively. To examine their application as anion receptors by UV-Vis and  $^1\text{H}$  NMR spectroscopy results revealed their higher selectivity for fluoride ion than other anions. The receptors and fluoride ion formed a 1:1 stoichiometry complex through strong hydrogen bonding interactions in the first step, followed by a process of deprotonation in presence of an excess of  $\text{F}^-$  in DMSO solvent.

일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: IV-ANAL.P-95

발표분야: 분석화학

발표종류: 포스터, 발표일시: 금 15:00~17:00

## Fluorescent Film Sensor for $\text{Zn}^{2+}$ ion via Monolayer Assembly of Receptor on Quartz Plate Surfaces

김관걸, 이은빈, 김동완, 김재상

경상대 화학과

Fluorescent self-assembled monolayers (SAMs) on hydrophilic oxide surfaces are developed as new sensing materials for metal ions. This fluorescent film sensor was designed and prepared by chemically immobilization of a terminal silane group of monomer molecule onto SAM on quartz plates and was used for detection of  $\text{Zn}^{2+}$  ion in MeOH solvent. The advantages of this technique have been demonstrated experimentally by the sensitive response of the presence of trace amount of  $\text{Zn}^{2+}$  in MeOH ( $\text{DL} = 1.7 \times 10^{-5} \text{ mol} \cdot \text{L}^{-1}$ ). Further experiments showed that the commonly encountered interfering substance have no interference to the process. A Fluorescent film were fully characterized using scanning electron microscope (SEM), Atomic force microscopy (AFM), X-ray photoelectron spectra (XPS), UV-Visible absorption and fluorescence measurements. Optical spectroscopy study of the film showed that strong interactions occur between the receptor molecule and  $\text{Zn}^{2+}$ . The position  $\lambda_{\text{max}}$  of the film shifts from 405 nm to 365 nm in methanol. Also the film emission intensity are increased at 486 nm due to intra-molecular charge transfer (ICT) in the excited state of the ionophore while the other transition metal ions showed little or no interaction. In conclusion, the super sensitive response and interference free of the sensing process, make the film a promising  $\text{Zn}^{2+}$  sensor.

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장소: 제주ICC

발표코드: IV-ANAL.P-96

발표분야: 분석화학

발표종류: 포스터, 발표일시: 금 15:00~17:00

## The Electropolymerization of Schiff-base Derivative with Terthiophene Units and Its Application as ISEs

김동완, 김관겸, 이은빈, \*황재영, 김재상

경상대 화학과 \*경상대 그린에너지융합연구소

A composite glassy carbon (GC) electrodes modified with bis(terthiophene)-appended schiff-base derivative (PTS) was used as solid state-ion selective electrode for determination of heavy metal ions. The electropolymerization of monomer (TS) onto GC was accomplished from the 1 mM TS in 0.1 M TBAP. The electrode displayed Nernstian response with slope of 29 mV decade<sup>-1</sup> in solution of pH 3-5. The limit of detection for electrode was  $3 \times 10^{-6}$  M with response time of 20 s. The electrode was also suitable as an indicator electrode in the potentiometric titration of Hg<sup>2+</sup>.

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장소: 제주ICC

발표코드: IV-ANAL.P-97

발표분야: 분석화학

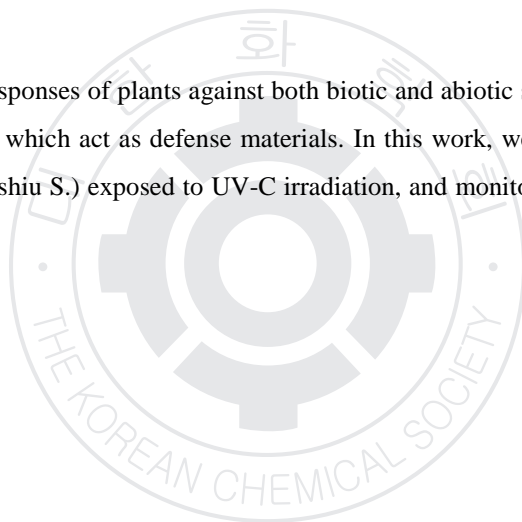
발표종류: 포스터, 발표일시: 금 15:00~17:00

## **Influence of UV stress on the changes of flavonoids in citrus peel**

정성우, \*이정환, \*박세민, \*서은누리, \*신성철

경상대 원예학과 \*경상대 화학과

In general, the protective responses of plants against both biotic and abiotic stresses have been associated with secondary metabolites which act as defense materials. In this work, we characterized flavonoids in the peel of citrus (*Citrus unshiu* S.) exposed to UV-C irradiation, and monitored their content changes by LC/MS-MS methods.





일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: IV-ANAL.P-98

발표분야: 분석화학

발표종류: 포스터, 발표일시: 금 15:00~17:00

## Depth profiling of non conducting coatings on a glass substrate

윤장희, 원미숙

한국기초과학지원연구원 부산센터

The radiofrequency glow discharge optical emission spectrometry (RF-GDOES) was used for a depth profiling of various non conducting coatings on a glass substrate. The technique permitted a rapid, and accurate elemental depth information of multi layered coatings on a non conducting substrate. The use of a RF source for sputtering permits the technique to be extended to applications of GD-OES to the study of conductors, semiconductors and insulators. This constitutes its main advantage compared to the better-known GD direct current (dc) counterpart. The analytical parameters were optimized for the RF-GDOES depth quantitative analysis. We extended the surface analytical capability to the accurate and rapid depth profiling of semiconducting films (Sn/Ag/Sn, CIGS/Mo), and polymer (Xylene) coating on a glass.

일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: IV-ANAL.P-99

발표분야: 분석화학

발표종류: 포스터, 발표일시: 금 15:00~17:00

## Identification of archaeological dyes and fabrics using FTIR and DF-UV/VIS/NIR

andrea ceglia, 이연희

KIST 특성분석센터

The textile research is of growing interest within archaeology because of its potential to provide relevant information either regarding the development and the technological advancement of ancient populations or the socio-economic and religious purposes of textile production. It is of paramount importance in the cultural heritage research to use non-destructive techniques; therefore, here it is proposed the use of FTIR and Diffuse Reflectance UV/VIS/NIR spectroscopy for the characterization of ancient textiles excavated in South Korea. In order to build a database, standard samples of dyed silk were prepared using several natural and synthetic dye compounds, which were analyzed with FTIR and DF-UV/VIS/NIR spectroscopy. FTIR spectra were recorded also for the dyes in powder to obtain the fingerprint of the pure dyeing materials. Afterwards spectroscopic analyses were carried out on 5 textiles fragments coming from XVI-XVIII century Korean tombs and the results give precious accounts concerning the burying rituals. FTIR and DF-UV/VIS/NIR spectra allowed the identification of fiber of the archaeological textiles, distinguishing between the cellulosic and the silk ones. Furthermore, it was possible to identify indigo in three blue fabrics and to show its presence in a green textile. The results suggest that FTIR and DF-UV/VIS/NIR are two efficient techniques very helpful for the characterization of excavated fabrics both dyed and natural.

일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: IV-ANAL.P-100

발표분야: 분석화학

발표종류: 포스터, 발표일시: 금 15:00~17:00

## **Analysis of the adsorption and desorption properties of xylene-imprinted polymer films using surface plasmon resonance technique**

장성우, \*유연규, 박찬량

국민대 화학과 \*국민대 생명나노화학과

We applied molecularly imprinted polymer thin films to the sensing of gaseous m-xylene and characterized the performance of gas sensing using surface plasmon resonance technique. The molecularly imprinted polymer films were synthesized by photo-polymerization method using several different templates, functional monomers and cross-linkers. The morphology and porosity of the polymer films were controlled using different mixing ratios of the pre-polymerization solution and confirmed by atomic force microscopy. The effects of templates and cross-linkers were interpreted by fitting the adsorption/desorption sensorgrams of gaseous m-xylene to the conventional kinetic models. The sensitivity and selectivity of sensor films were estimated against humidity and other gaseous molecules such as formaldehyde and ammonia.

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장소: 제주ICC

발표코드: IV-ANAL.P-101

발표분야: 분석화학

발표종류: 포스터, 발표일시: 금 15:00~17:00

## Osmanthus heterophyllus(구골나무)의 꽃의 아로마 성분 분리와 향산화 효과

주성진, 김일광

원광대 생명나노화학부

Osmanthus heterophyllus(구골나무)의 꽃을 채취하여 아로마 성분을 분석하였다. methanol 과 hexane (1:2)로 추출하고 용매극성을 달리 하면서 용매분리를 진행하였다. Butanol 층을 감압농축하고 실리카겔 칼럼에서  $\text{CHCl}_3$ -MeOH-H<sub>2</sub>O(50:10:1 → 10:10:1)조건으로 분리하였다. PEG-20M, 캐필러리 Chiramix 칼럼을 사용하는 GC-Mass 에서 linalool, furanoid, decalactone 등을 확인하였으며, 이들의 향산화 효과결과를 비교하였다.

일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: IV-ANAL.P-102

발표분야: 분석화학

발표종류: 포스터, 발표일시: 금 15:00~17:00

## **A role of arginine methylated Lamin A/C during myoblast fusion**

김수진, 이상원

고려대 화학과

Protein arginine methylation has been implicated in the pivotal regulation of cellular events such as RNA processing, transcriptional regulation, signal transduction, insulin secretion, and DNA repair. A recent report showed the involvement of protein arginine methyltransferase (PRMT) 4 in chromatin remodeling and gene expression during muscle differentiation in C2C12 cells. As the fusion of myoblasts is a unique phenomenon observed in skeletal muscle differentiation, the present report focused on the expression and activities of PRMTs during myoblast fusion in primary rat skeletal muscle. NG, NG-asymmetric dimethylarginines (aDMA) and NG, N'-G-symmetric dimethylarginines (sDMA) were both found consistently throughout myoblast fusion. However, PRMT1 exhibited the highest activity during myoblast fusion and maintained the elevated activity thereafter, whereas PRMT5 reached its highest activity only after myoblast fusion. To identify the proteins modified by such PRMTs, we conducted 2-dimensional electrophoresis (2-DE) of total proteins before and after myoblast fusion, and protein spots on the 2-DE gel immunoreactive for aDMA and sDMA were identified by mass spectrometric analysis. Among the proteins identified, lamin C2 was in particular observed to be dimethylated. Arginine methylation of lamin may therefore be important for muscle development and maintenance.

일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: IV-ANAL.P-103

발표분야: 분석화학

발표종류: 포스터, 발표일시: 금 15:00~17:00

## Simultaneous determination of benzoic acid and sorbic acid in food products by capillary electrophoresis after on-line preconcentration by dynamic pH junction

zhang xinfeng, \*Shuxia Xu, \*Yanyan Wang, 임재민, 이용일

창원대 화학과 \*College of material and chemistry & chemical engineering, Chengdu university of Technology, Sichuan, Chengdu 610059, China

Benzoic acid (BA), sorbic acid (SA) and their salts are the permitted chemical preservatives in food products to prevent transformation and degradation by microorganisms during storage. However, BA and SA may be harmful to consumers in case of excessive addition [1, 2]. In this work, an on-line dynamic pH junction method has been proposed for sensitive determination of benzoic acid (BA) and sorbic acid (SA) by capillary electrophoresis (CE). It was based on the decreased mobility of the analytes when it migrated from sample zone with low pH to background electrolytes (BGE) with high pH. Fig. 1 shows the effects of injection time on the preconcentration and CE separation. Under optimized conditions, the limits of detection (S/N=3) of BA and SA were 0.03 mg/L and 0.02 mg/L, respectively. According to the permitted limits of BA and SA in food (GB2760), the samples can be diluted about 2000-20000 folds to estimate whether the contents of BA and SA are in the safety range. Beverage, vinegar and fruit jam samples were analyzed after simple dilution, and the results were satisfactory with the recoveries in the range of 91-108%. The whole analysis process needs about only 10 min, which is much faster than the method of liquid-liquid extraction followed by CE determination.

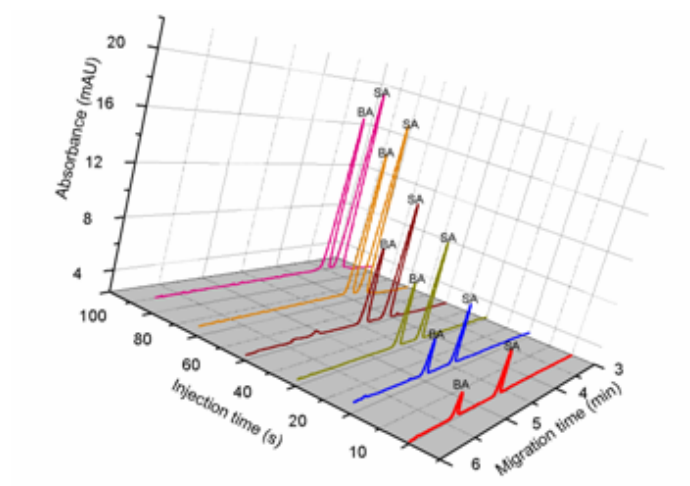


Fig. 1. Effects of injection time on the preconcentration and CE separation



일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: IV-ANAL.P-104

발표분야: 분석화학

발표종류: 포스터, 발표일시: 금 15:00~17:00

## **Gold nanodendrite structure as an effective SERS substrate**

신가영, 정희일

한양대 화학과

Recently, diverse noble metal nanostructures have been demonstrated as a promising SERS (Surface Enhanced Raman scattering) substrate. In particular, dendrite structures could attract large attention since these can generate many hot-spots inside the structure and the synthesis is relatively easy and reproducible, such as by simple electrodeposition. In this study, we fabricated gold nanodendrite network porous structure by an electrochemical method. The nanodendrite network porous structure was constructed on a platinum surface through electro-deposition of Au under the presence of hydrogen bubbles generated from the same surface. Iodide, used as a co-reagent, played an important role in the construction of the nanodendrite network by preventing continual growth of Au into larger agglomerates as well as inhibiting coalescence of neighboring nanodendrites. Using the nanodendrite network structure, 2-naphthalenethiol was applied on it and the corresponding SERS spectra were collected. Finally, optimal conditions for synthesis providing maximum SERS intensity have been investigated and the resulting structure was characterized.



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장소: 제주ICC

발표코드: IV-ANAL.P-105

발표분야: 분석화학

발표종류: 포스터, 발표일시: 금 15:00~17:00

## Evaluation of the Analytical Performance of Near-Infrared (NIR) Micro-Spectrometer

신가영, 정희일

한양대 화학과

The major purpose of this study is to develop a near-infrared (NIR) micro-spectrometer using a light emitting diode (LED) as a light source. A linear variable filter (LVF) and diode array detector were integrated for wavelength selection and radiation detection, respectively. Furthermore, it was constructed for dual channel configuration, in which the reference and sample spectra can be collected simultaneously. The most important advantage of this design is to acquire reliable baseline stability by continuous referencing to the reference channel. The micro-spectrometer is capable of collecting spectra in the 5000-4000  $\text{cm}^{-1}$  range where the most sensitive NIR bands can be utilized for qualitative and quantitative analysis. The analytical performance of this prototype micro-spectrometer was evaluated, through the analysis of binary and tertiary liquid sample mixtures. In parallel, NIR spectra of these samples were collected using a commercial FT-NIR spectrometer for comparison.

일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: IV-ANAL.P-106

발표분야: 분석화학

발표종류: 포스터, 발표일시: 금 15:00~17:00

## Quantitative Analysis of D/L-amino Acid with Derivatization by ESI-Q-TOF Mass Spectrometry using Kinetic Method

진광재, 임재민, 이용일

창원대 화학과

A novel method was developed for quantitative determination of D/L-amino acids based on the derivatization and subsequently analysis by electrospray ionization quadrupole time-of-flight mass spectrometry (ESI-Q-TOF-MS) using kinetic method. The amino acid enantiomers were first modified by the commonly used derivatization reagent, N,N-Dimethylformamide dimethyl acetal (DMF-DMA), under the optimized condition within an precisely temperature-controlled oven. Then the resulting derivative and a pre-mixed solution containing an appropriate transition metal ion and a reference ligand were simultaneously injected, by using T-union, to MS system to generate singly charged transition metal ion-bounded clusters by electrospray ionization in the gas phase. The precursor cluster ion of interest was mass-selected and the kinetics of its competitive unimolecular dissociations was investigated in a quadrupole time-of-flight mass spectrometer under MS/MS mode for kinetic method study. Their characteristic mass spectrometric fragmentation patterns were studied and the corresponding fragmentation pathways were proposed. Quantitative determination of the enantiomerically compositions of the D/L-amino acids were achieved by using constructed calibration curves. The derivatization was assumed to improve the chiral selectivity, which accordingly contribute to the improvement of quantitative analysis. Keywords: D/L-amino Acid, ESI-Q-TOF-MS, DMF-DMA, Derivatization, Kinetic Method

일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: IV-ANAL.P-107

발표분야: 분석화학

발표종류: 포스터, 발표일시: 금 15:00~17:00

## **New matrix of mesoporous materials and its application in MALDI-TOF mass**

**jia biao, \*Donghao Li, 임재민, 이용일**

창원대 화학과 \*Instrumental Analysis Center, Yanbian University, Yanji 133002, China

The matrix effect of mesoporous silica sba-15 and sba-15NA with a small organic molecular were mainly investigated in this work using MALDI-TOF-MS. For MALDI-TOF-MS analysis of low molecular weight compounds, compared with a conventional matrix, mesoporous silica exhibited less background interference ions, a high desorption/ionization efficiency, high homogeneity and good reproducibility. This also offers a new technique for fast analysis of oligosaccharides, amino acids, drugs and polymer characterization, indicating mesoporous materials that have good versatility. The modified sba-15NA appeared to be an outstanding matrix for analytes, suggesting that functionalized organic molecular have a great effect on novel matrix for MALDI-TOF MS analysis.

일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: IV-ANAL.P-108

발표분야: 분석화학

발표종류: 포스터, 발표일시: 금 15:00~17:00

## **Analysis of low frequency Raman spectra of zearalenone and its derivatives.**

강원석, 안대희, 연찬미, 성소희, 김재호

아주대 분자과학기술학과

Low-frequency Raman spectroscopy provides information on local structure of solutions coupled with hindered translational and librational motions. Zearalenone (ZEN) is a mycotoxin produced by several species of the genus *Fusarium*, mainly *Fusarium graminearum*. This mycotoxin and its derivatives (Zearalanone(ZAN), Zearalenol(ZENOL), Zearalanol(ZANOL)) are frequent contaminants of cereal crops, such as maize, barley, oats, wheat and other grains throughout the world. For this reason, many countries of the world have established maximum tolerance ranges of these mycotoxins from 30 to 1000 g/kg in grains. In this study, Raman spectroscopic technique which is well known as a non-destructive analytical tool for the in situ identification of both organic and inorganic materials, was used to characterize the ZEN and its derivatives. Raman spectra were collected using a triple monochromator coupled with a CCD array detector (Tripletmate 1877, Spex Industries, Edison, NJ, USA). And laser power for all experiments was used 15 mW at 514.5 nm (Innova 70 Ar+ laser, Coherent Co., CA., USA). We report low frequency Stokes Raman spectra in the range between 30 and 200 cm<sup>-1</sup>.

일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: IV-ANAL.P-109

발표분야: 분석화학

발표종류: 포스터, 발표일시: 금 15:00~17:00

## A Simple Method for $^{18}\text{O}$ Stable Isotope Labeling for the Quantification Analysis in MS-based Proteomics

이정화, 정희정, 문동기, 김호근, 이상원

고려대 화학과

A variety of stable isotope labeling techniques have been developed and used in shotgun proteomics for relative peptide/protein quantitation in mass spectrometry (MS)-based analysis. Trypsin-catalyzed isotope  $^{16}\text{O}/^{18}\text{O}$ -labeling of the C-terminal carboxyl group of peptide is gradually used more and more, but this methodology still has a limitation that the quantitative measurements are often inaccurate when remaining trypsin that can catalyze the back exchange of  $^{18}\text{O}$  with  $^{16}\text{O}$  after labeling. We demonstrate a means to minimize postlabeling back exchange when peptides are used to analyze for an ongoing proteomics study. For completely quenching, the sample was boiled, acidified and filtrated to remove the residual trypsin using a membrane filter. Finally, the Liquid Chromatography (LC) MS analysis results were evaluated against simulated composite  $^{16}\text{O}/^{18}\text{O}$  ratio spectra where peptide molecular weight and  $^{16}\text{O}/^{18}\text{O}$  ratio. Based on analysis results, we described an improved  $^{18}\text{O}$ -labeling protocol by using solution-phase trypsin. The means to generate stably  $^{18}\text{O}$ -labeled samples without back-exchange should enable more effective applications of  $^{18}\text{O}$ -labeling toward large-scale biomarker discovery where an  $^{18}\text{O}$ -labeled sample can be used as a reference for quantitation.

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발표코드: IV-ANAL.P-110

발표분야: 분석화학

발표종류: 포스터, 발표일시: 금 15:00~17:00

## Analysis of aflatoxins using MWCNT as an aflatoxin adsorbent by LC-MS/MS

이동욱, 권종은, 이계호

충남대 화학과

곰팡이독소는 *Aspergillus*, *Penicillium* 과 *Fusarium* 속 등의 유해곰팡이에 의해서 생성되는 2 차 대사산물로서 포유동물인 인간과 동물에 유해한 작용을 나타내는 유독물질을 총칭한다. 주로 옥수수, 수수, 보리등과 같은 곡물과 농산품 전반에 걸쳐 발견이 되며, 수확 전·후 또는 수송이나 보관 중에 발현이 되고, 대부분 비교적 안정된 화합물이므로 사료의 가공공정을 통하여 파괴되지 않으며, 제분을 통하여 농축이 되어 질 수도 있다. 현재 약 300~400 종류의 곰팡이독소가 알려져 있으나 식품이나 사료 등에 존재하면서 잠재적으로 사람의 건강에 유해한 영향을 줄 수 있는 곰팡이독소는 약 10~20 종류이다. 그 중 *Aspergillus* 속 균이 생산하는 aflatoxin 은 강력한 발암물질로서, IARC(International Agency for Research on Cancer)에 의해 인체발암물질을 뜻하는 Group 1 으로 지정이 되었으며, 이에 오염된 식품이나 사료를 섭취한 사람이나 동물에게 여러 가지 장애를 일으키고, 특히 간암이나 식도암 등의 발암성과 관련이 있기 때문에 세계 각국에서 MRLs(Maximum Residue Levels)을 지정하여 규제를 하고 있는 실정이다. 최근 아플라톡신 분석에 있어 Immunoaffinity column 의 항원 항체 반응을 이용하여 아플라톡신만 선택적으로 결합을 시켜서 분석하는 방법이 시행되고 있다. Immunoaffinity column 이 아플라톡신을 선택적으로 결합하는 충진물인 항체를 만드는데 있어서 비용이 많이 들기 때문에 Immunoaffinity column 의 가격이 비싸다. 이러한 이유로 최근 연구는 Immunoaffinity column 대신에 가격이 저렴하면서 아플라톡신만 선택적으로 분석하는 연구가 진행되어지고 있다. 이에 우리는 MWCNT 의 아플라톡신 흡착 능력을 이용하여 흡착시킨 후 탈착을 시킴으로써 아플라톡신을 선택적으로 분석을 수행할 수 있었고, 기존의 Immunoaffinity column 보다 용매의 사용이 적고, 시간이 적게 걸리며 경제적으로 저렴한 분석방법을 개발하였다.

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발표코드: IV-ANAL.P-111

발표분야: 분석화학

발표종류: 포스터, 발표일시: 금 15:00~17:00

## Multiresidue method for determination of pesticides in Tea samples using dispersive solid-phase extraction by LC-MS/MS

김소연, 이동욱, 이계호

충남대 화학과

우리가 과거에 식품의 질과 맛의 향상을 위해 사용되었던 화학 물질의 문제가 부각되자, 여러 국가에서 국민의 건강을 위해 이를 규제하고 연구를 진행하고 있다. 특히, 농산물의 농약사용과 관련하여 각국의 상황에 맞게, MRL(Maximum Residue Levels)을 규정하여 규제하고 있다. 최근, 세계 곳곳에서 차 문화에 대한 관심이 커지며 우리나라에서도 많은 이들이 다양한 차를 즐기고 있는데, 이에 대한 재배과정에서의 농약처리에 대해서는 알고 있는 사실이 적다. 따라서 대중화된 차의 잠재적으로 함유되어 있는 농약에 대한 정보가 현대인에게 정확하게 인식되어야 된다. 이번 실험을 통해 alkaloids 나 polyphenol, pigments 등의 복잡한 matrix 를 갖고 있는 차 분석에 적합한 추출과정의 최적화와 다성분 농약의 동시분석을 가능하게 하는 분석방법의 최적화를 이용하여 잔류농약 분석 분야의 발전을 도모하고자 했다. 본 실험에서는 liquid chromatography 와 질량분석기로 tandem mass spectrometry 를 이용하여 다성분 농약 동시 분석을 진행하였다. 실험 과정에서, tea samples 에 표준적으로 적용 가능한 추출용매로 acetic acid 를 포함한 acetonitrile 을 이용하였고, tea 속의 다양한 matrix 제거를 위한 방법으로 DSPE (dispersive solid phase extraction)을 cleanup 과정으로 이용하기 위해서, PSA, C<sub>18</sub>, GCB 등의 DSPE sorbents 에 대한 최적화 실험을 진행하였고, 이에 대한 method validation 을 하였다.

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장소: 제주ICC

발표코드: IV-ANAL.P-112

발표분야: 분석화학

발표종류: 포스터, 발표일시: 금 15:00~17:00

## Analysis of aflatoxins and ochratoxin A by dispersive solid-phase extraction in LC-MS/MS

권종은, 이동욱, 이계호

충남대 화학과

Mycotoxin 은 곰팡이가 생산하는 2 차 대사산물로서 사람과 가축에 질병이나 이상생리작용을 유발하는 물질이다. 그 중 *Aspergillus* 속 곰팡이에 의해 생성되는 Aflatoxin(AFT)과 Ochratoxin A(OTA)는 강한 독성 때문에 전 세계적으로 관심을 받고 있는 곰팡이 독소이다. 때문에 대부분의 나라에서는 이들에 대해 MRLs(maximum residue levels)를 정하여 규제를 하고 있다.

Aflatoxin(AFT)과 Ochratoxin A(OTA)는 곡류와 견과류, 저장된 건조식품 등에서 많이 발견되고 있다. 곰팡이독소 대부분은 고온다습하거나, 건조되지 않은 농산물에서 잘 발견된다. 이는 식량에서의 곰팡이독소 발견문제와 바로 관련이 되기 때문에 곰팡이독소에 대해 빠르고 정확한 분석법이 필요하다.

공전법에서 주로 쓰이는 immunoaffinity column(IAC)은 항원-항체 반응을 이용하기 때문에 선택성이 좋은 장점이 있지만, 선택적으로 결합하는 항체를 이용하기 때문에 비용이 많이 들고 많은 시간과 유기용매의 사용 또한 필요하게 된다.

이에 비해 좀 더 경제적이고 동시분석을 할 수 있는 방법으로, QuEChERS(Quick, easy, cheap, effective, rugged, safe)방법이 있다. 이 방법의 clean up 과정에서는 DSPE(dispersive solid-phase extraction) 방법을 사용하는데, 이 과정에서는 흡착제를 분산시킴으로써 유기용매의 사용과 분석시간을 최소화할 수 있다.

이 실험에서는 DSPE 방법을 이용하여 AFTs 4 종(AB1, AB2, AG1, AG2)과 OTA 에 대해 빠르고 간편한 분석방법을 발전시켰다.



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장소: 제주ICC

발표코드: IV-ANAL.P-113

발표분야: 분석화학

발표종류: 포스터, 발표일시: 금 15:00~17:00

## **Optical investigation on sensitivity enhancement of the trigonal-pyramid Surface Plasmon Resonance sensor chips fabricated by Langmuir-Blodgett technique**

연찬미, 성소희, 강원석, 김재호

아주대 분자과학기술학과

The surface plasmon resonance (SPR) has been widely employed for biosensor applications because of the capability for label-free detection of biomolecular interactions. However, the sensitivity of SPR sensor is lower than the conventional labeling immuno-sensing methods. The metal nanostructure-amplified surface plasmon resonance analysis has been investigated to enhance the sensitivity. We used trigonal pyramid Au nanostructured SPR chips for SPR sensitivity enhancement and took a theoretical approach by evaluating optical properties of the Au-nanostructures and nanostructured SPR chips in the point of localized surface plasmon (LSP)- surface plasmon polariton (SPP) conjugation. We used the Langmuir-Blodgett (LB) method for preparation of defect-free and large-area silica-nanoparticles-monolayer as a template for the fabrication of nano-scaled Au patterns on an Au substrate for surface plasmon resonance. Well organized, trigonal pyramid shaped Au nano-structures were able to construct on 34 separate chips in one fabrication process. The dimensions of trigonal pyramid nano-structures were precisely controlled by changing the particle diameter of the silica LB template as follows: 150, 300, 500, and 700 nm. The nano-structure patterned substrate fabricated with 300 nm-sized silica nanoparticles demonstrated a sensitivity enhancement up to 120 % compared to a conventional SPR chip when 20% aqueous ethanol solution was used as an analyte. To improve the optical basis of the enhancement in the sensitivity, we measured the SPR curves to wavelength. Also we tried to measure UV-visible spectra of the Au nanostructured pattern in the attenuated total reflectance (ATR) mode to observe the LSP mode of each Au nanostructure.

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장소: 제주ICC

발표코드: IV-ANAL.P-114

발표분야: 분석화학

발표종류: 포스터, 발표일시: 금 15:00~17:00

## **A Column Temperature Controllable Ultra-high Pressure Liquid Chromatography (UPLC) System: Effects and Potentials on Proteomic Study**

문동기, \*이후근, 이상원

고려대 화학과 \*가천의과학대 암당뇨연구원

The temperature is regarded as a universal physicochemical parameter factor in chromatography. Temperature control in chromatography exhibited several chromatography benefits such as reduction in analysis time, changes in selectivity of analytes, and increase in separation efficiency. Despite these advantages, the temperature control system is not universally used in proteomics, mainly due to the technical difficulties to incorporate the temperature control module, especially for the analysis of peptides using a long microcapillary column with electrospray ionization (ESI) interface. In this study, the temperature controlling device allowed precise temperature control of a microcapillary column longer than 70 cm up to 60 °C with a simple incorporation of a semi-rigid gasline heater. The tryptic enolase peptides were used as a standard sample to evaluate the effect of the temperature control on the peptide separation efficiency and reproducibility. In addition to the increased reproducibility in peptide elution time by the temperature control, the temperature elevation resulted in decrease of column operation pressure, which allowed employing higher solvent flow-rate for the same LC pumps and led to further improvements in  $\mu$ LC performances.

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발표분야: 분석화학

발표종류: 포스터, 발표일시: 금 15:00~17:00

## Separation mechanism of polycyclic aromatic hydrocarbon mixtures on seven kinds of $\pi$ -acidic or $\pi$ -basic stationary phases

정영한, \*류재정, \*\*남궁현, \*\*\*권소연

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C18 column is commonly used for analysis of PAH (polycyclic aromatic hydrocarbon) mixed samples by reverse phase HPLC mode. In this study, seven kinds of  $\pi$ -acidic or  $\pi$ -basic stationary phases are used for separation of the  $\pi$ -electron rich PAH mixed samples by normal phase HPLC mode. As results, a  $\pi$ -acidic functional group, DNB (dinitrobenzoyl) group containing stationary phases show better result than a  $\pi$ -basic functional group, DMB (dimethylbenzoyl) group containing stationary phases and phenyl group roles more importantly than iso-butyl or tert-butyl group in the resolution of PAH mixture. Therefore, both face to face and face to edge  $\pi$ - $\pi$  interaction are important in this resolution. In addition, a DNB group containing octadecyl silane (ODS or C 18) stationary phase shows a good resolution of PAH mixture in comparison with the result from commercial ODS column.

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장소: 제주ICC

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발표분야: 분석화학

발표종류: 포스터, 발표일시: 금 15:00~17:00

## **Sensitivity enhancement of Ag/Au Bilayer for ethanol sensor by Surface Plasmon Resonance Ellipsometry method**

성소희, 연찬미, 강원석, 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. Gold is the most general material in SPR sensor for its chemical stability and capability of biomolecule adhesion, but SPR sensor based on gold film had lower sensitivity compared with silver film. Silver is a good material for SPR sensing because of its high SPR excitation efficiency leading to high sensitivity, but it generates unstable signal due to its oxidation in natural condition. Generally, there are three virtues of using SPR ellipsometer for biosensing. First, the maximum phase difference and the minimum ratio of reflection coefficient in SPR condition. Second, Sensitivity of the resonance conditions are most sensitive in the characterization. Third, SPR ellipsometry is more sensitive than reflectometry. In this study, we used Ag/Au bilayer for SPR sensitivity enhancement. Ag/Au bilayer was fabricated by e-beam evaporation on the flat  $18 \times 18 \text{ mm}^2$  cover glass substrates. The results show that in comparison to conventional flat Au chips, sensitivity enhancement decreases in angular mode. However, the Ag/Au bilayer signal using SPR ellipsometer demonstrated a sensitivity enhancement up to 160% compared to a conventional SPR chip.

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발표종류: 포스터, 발표일시: 금 15:00~17:00

## Carbon Nanotube Based Schottky Device as a Highly Sensitive Biosensor

안대회, 김재호

아주대 분자과학기술학과

Single walled carbon nanotubes (SWNTs) have been widely studied due to its potential applications in various fields, such as field-effect transistor, flexible transparent electrode, chemical sensor and probe tip. Especially, SWNT based biosensor has attractive advantages of label-free detection, higher sensitivity and miniaturized device. In order to make device SWCNT film was fabricated by Langmuir-Blodgett (LB) technique. Unidirectionally aligned LB film shows pseudo-metallic property and its lowers the barrier between gold electrodes and CNT film. Low barrier allows electrons to move easily from source to drain, which causes the poor sensitivity of the device. However, this problem can be solved by using large center position gold as a sensing area. Many probe biomolecules strongly adsorbed on gold surface by self assembly. When biotin molecules immobilized on gold surface current was subsequently decreased with addition of more high concentration of streptavidin molecule. Schottky device current was modulated by gold work function and it was also affected by injected target biomolecules. Detection limit of our device is 100 pM in streptavidin detection experiment. Real clinical serum based human immunodeficiency virus (HIV) was also detected using our device in PBS buffer solution (pH 7.4). Non specific binding was not occurred in BSA solution (0.1  $\mu$ M) and the current was gradually decreased with injection of HIV antibody solutions.

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## Simultaneous determination for pesticides in Natural Herbs by gas chromatography mass spectrometry

안영웅, 이동욱, 이계호

충남대 화학과

최근 들어 유기농 허브를 이용한 여러 제품들이 많이 생산 되고 있다. 이런 유기농 허브 추출물들은 화장품 제조에 사용하거나 기능성 음료에 첨가 하고 있다. 때문에 직접적으로 피부에 접촉하거나 음용하게 된다. 따라서 유기농 허브가 잔류 농약에 노출되어 있다면 그 위해성은 무척 크다. 그러므로 유기농 허브에 대한 잔류 농약의 분석은 필요하며 그것을 통하여 소비자들을 잔류 농약에 의한 위해성으로부터 지켜 줄 것이다. 현재 식품 중에 잔류하는 농약에 대해서 세계 각국에서는 농약에 대한 MRL(Maximum Residue Levels)을 지정하여 규제를 하고 있는 실정이다. 이 실험에서는 유기농 허브를 시료로 이용하여, acetonitrile 를 이용하여 추출 시키고, PSA 와 GCB 를 사용한 Dispersive-SPE 방법을 사용하여 경제적이고, 빠르며 많은 시료에 대해 쉽게 전처리를 할 수 있었다. 또한 GC/MS 이용하여 다성분 동시분석을 할 수 있는 분석법을 확립하였다. matrix 에 대한 효과를 줄이기 위해 matrix matching calibration 을 하였고, 최적화된 전처리 방법과 기기조건을 찾아내었다. 본 실험을 통하여 최적화된 전처리 방법을 개발하여 여러 가지 시료와 분석 물질에 적용함으로써 앞으로 선진국의 농약 잔류 기준에 한 발 더 다가가고, 동시에 다성분을 짧은 시간에 분석하는 조건을 확립하게 되었다.

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발표종류: 포스터, 발표일시: 금 15:00~17:00

## SERS-based Immunoassay on a Disk Using Hollow Gold Nanospheres

전향아, \*이상엽, 추유진, \*\*황현두, \*\*조윤경, 주재범

한양대 바이오나노공학과 \*한양대 응용화학과 \*\*울산과학기술대 나노생명화학공학부

A sensitive and reproducible surface-enhanced Raman scattering (SERS)-based immunoassay technique, using hollow gold nanospheres (HGNs) and glass beads, has been developed for blood samples analysis. Here, the innovative laser irradiated ferro wax microvalves and centrifugal microfluidics were utilized for the full integration of glass bead-based suspension SERS based immunoassays on a disc starting from whole blood. Glass beads and hollow gold nanospheres were used as supporting substrates and SERS probes for the formation of the immunocomplex. All the necessary reagents are preloaded on the disc and the total process of the plasma separation, incubation with target specific antigen- or antibody-coated microbeads, multiple steps of washing, probe reaction with substrates, and the indirect Raman detection could be finished within 30 minutes. Moreover, no special skills are necessary. For the validation of our SERS immunoassay, well-known cardiac markers such as troponin I, myoglobin and creatine kinase-myoglobin (CK-MB) were used as target markers.

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장소: 제주ICC

발표코드: IV-ANAL.P-120

발표분야: 분석화학

발표종류: 포스터, 발표일시: 금 15:00~17:00

## Highly Robust Label-Free Quantitation Platform for LC-MS/MS Analysis Based on Master AMT DB (Accurate Mass and Time Database)

정희정, 김호근, 문동기, 김수진, 이상원

고려대 화학과

One of the most important purposes of proteomics is to accurately quantify protein changes in various biological conditions. Although label-free approach outperforms labeling methods in the aspects of throughput, simplicity of experimental procedure, and cost, a robust and elaborate data processing platform is critical to achieve more accurate quantitation by label-free approach. We present a highly robust label-free quantitation analysis platform for LC-MS/MS experiments based on the Master AMT DB. Assigning accurate monoisotopic precursor masses to tandem mass spectrometric data is a critically important step for successful peptide identifications from LC-MS/MS experiments. iPE-MMR was developed for this and demonstrated for improving accuracy in peptide identification. Accurate time tag is enabled by applying temperature controlled system to improve reproducibility in LC-MS/MS experiments and introducing normalized elution time (NET) method to minimize chromatographic variation. Peptide identification was done through SEQUEST and validated using target-decoy method. These peptides were used to assemble Master AMT DB. In this step false-positives were decreased by applying experimental cross correlation (E-Xcorr) scoring, a pattern matching scoring routine between MS/MS spectra for each peptide. The unassigned MS features through SEQUEST searches could be additionally assigned by matching it to Master AMT DB under optimized mass and NET tolerance. E-Xcorr also could be applied to confirm the newly assigned peptide if the MS feature had corresponding MS/MS spectra. Finally peptide abundance was aligned sample to sample and normalized. Protein quantity was evolved through statistical test which provide clues to find potential biomarker candidates.



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장소: 제주ICC

발표코드: IV-ANAL.P-121

발표분야: 분석화학

발표종류: 포스터, 발표일시: 금 15:00~17:00

## **Simultaneous detection of two DNA markers using SERS-based gradient optofluidic sensor**

**최남현, 황준기, 이문권, 주재범**

한양대 바이오테크놀로지학과

In recent years, considerable progress has been made in the development of surface-enhanced Raman scattering (SERS)-based microfluidic system to detect chemical and biological analytes in fast and sensitive manner. Generally, microfluidic device for the SERS detection is composed of nanocolloid and microfluidic compartment. We present the application of the SERS method for a sensitive detection for duplex cancer marker genes in a gradient microfluidic channel. This technology does not need either an immobilization or amplification step and provides a rapid and sensitive detection of DNA markers. Herein, a gradient microfluidic channel was used to automatically generate the mixture of duplex DNA samples with different mixing ratio. By using this automatic mixture generation system, a tedious manual mixing process can be avoided and a fast and sensitive DNA analysis could be achieved under continuous flow. BRCA1 and BAX were used as target genes. BRCA1 is a gene overexpressed in breast cancer cells, and BAX is known to be closely related with their apoptosis. In this presentation, the application of SERS-based microfluidic sensor for highly sensitive cancer gene (BRCA1 and BAX) diagnostics will be introduced.

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장소: 제주ICC

발표코드: IV-ANAL.P-122

발표분야: 분석화학

발표종류: 포스터, 발표일시: 금 15:00~17:00

## Physicochemical Characterization and Sorption Capacity of Biochar generated by Hydrothermal Carbonization

배선영, 고은솔

서울여대 화학과

Biochar has received a great attention due to its useful applications such as alternative energy production, carbon sequestration or soil fertilization. Variation of feedstock and thermal processing conditions produces a distinctive physicochemical properties of biochar. In this study, hydrothermal carbonization of cabbage was performed in a tubular reactor at 150 °C and 220 °C for 30 min, 1.5 hr, and 2 hr to investigate the sorption capacity of biochar on heavy metal. The sorption experiment was conducted by using four different concentrations of Zn (2, 5, 8, 10 ppm) and various pH (from 5 to 8). The sorption isotherm results show that Zn sorption was favorable, spontaneous and increase in the pH ranges. To compare the surface areas, the iodine numbers of various biochars were determined, which were 32.5 ( $\pm 7.5$ ) mg/g for cabbage, 257.3 ( $\pm 17.4$ ) for biochar, 498.0 ( $\pm 5.5$ ) for the activated carbon, and 635.0 ( $\pm 12.6$ ) mg/g for the commercial activated carbon.

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장소: 제주ICC

발표코드: IV-ANAL.P-123

발표분야: 분석화학

발표종류: 포스터, 발표일시: 금 15:00~17:00

## Gold-array embedded gradient chip for SERS-based immunoassay

이문권, 최남현, \*윤지연, \*\*주재범

한양대 바이오 나노공학과 \*한양대 바이오 나노학과 \*\*한양대 생명나노공학과

This presentation introduces a novel immunoassay technique using a surface-enhanced Raman spectroscopy (SERS) and a gradient microfluidic channel. We designed and fabricated a 2-fold logarithmic gradient channel to generate various concentrations of a specific cancer marker. Furthermore, the Au film-coated glass substrate and hollow gold nanospheres (HGNS) were used for a highly sensitive SERS detection. The Au array surface was functionalized with carboxylic acid via self-assembled monolayer method using 11-mercaptoundecanoic acids. Then, the capture antibodies were immobilized on the carboxyl group-modified Au arrays through covalent bonding. HGNS, conjugated with specific Raman reporters and secondary antibodies, have been used for the SERS signal enhancement. We have employed this method for the quantitative analysis of a lung cancer marker, AFP ( $\alpha$ -feto protein), by forming self-assembled sandwich immunocomplexes onto Au arrays embedded micro-gradient channel. All aqueous solutions were precisely controlled by micro-syringes and infusion pumps. This conceptually new gradient chip-based immunoassay is expected to be a powerful tool for reliable and sensitive clinical diagnosis.

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장소: 제주ICC

발표코드: IV-ANAL.P-124

발표분야: 분석화학

발표종류: 포스터, 발표일시: 금 15:00~17:00

## **An NMR Study on the Polycarbonate and Poly(butylene terephthalate) Blends : Quantitative analysis and verification of trans-esterification reaction**

유효연, 천아영, 원다은, 서지혜, 안상두

중앙대 화학과

The basic properties of a polymer blend are influenced by those of its constituent monomers and the composition of component polymers. For that reason, it is important to analyze the composition of polymer blend correctly. In this study, we have firstly carried out the quantitative analysis for the PC/PBT blend using FT-IR, TGA, and NMR spectroscopy. Secondly, we have examined the trans-esterification reaction between polycarbonate(PC) and polybutylene terephthalate(PBT) by NMR because trans-esterification reaction can influence the properties of polymers such as miscibility, phase structure, crystallization, etc. especially for the polyester blends such as PC and PBT, To investigate the properties of the trans-esterification reaction and the effects of the inhibitor, NMR experiments were performed on two groups of samples with varying the annealing times. One is a commercial blend of PC and PBT with a small amount of inhibitor to the trans-esterification reaction, and the other is a simple mixture of PC and PBT without inhibitor. The experimental results show that the trans-esterification reaction increases as annealing time becomes longer.

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장소: 제주ICC

발표코드: IV-ANAL.P-125

발표분야: 분석화학

발표종류: 포스터, 발표일시: 금 15:00~17:00

## Investigation of the Local Micro-Structure of the $0.3\text{Li}_2\text{MnO}_3 \cdot 0.7\text{Li}[\text{Mn}_x\text{Ni}_y\text{Co}_z]\text{O}_2$ during Electrochemical Cycling by X-ray Absorption and $^7\text{Li}$ MAS NMR Spectroscopy

송혜영, 신병철, 이영일

울산대 화학과

Manganese-rich layered electrode materials, represented by the general formula  $x\text{Li}_2\text{MnO}_3 \cdot (1-x)\text{LiMO}_2$  in which M is Mn, Ni, and Co, are interesting for both high-power and high-capacity in lithium ion cells. Herein, the structural and electrochemical characterization have been performed for the  $0.3\text{Li}_2\text{MnO}_3 \cdot 0.7\text{Li}[\text{Mn}_x\text{Ni}_y\text{Co}_z]\text{O}_2$  as a function of x, y, and z. *In situ* X-ray absorption spectroscopy (XAS) has been used to study electronic and crystal structural changes during the first charge cycle. Also,  $^7\text{Li}$  MAS NMR spectroscopy has been performed for characterizing local structure in cathode materials with or without long-range order. In this study, the effect of Li deintercalation on the layer-structured  $0.3\text{Li}_2\text{MnO}_3 \cdot 0.7\text{Li}[\text{Mn}_x\text{Ni}_y\text{Co}_z]\text{O}_2$  has been systematically investigated by using *in situ* XAS and *ex situ*  $^7\text{Li}$  MAS NMR spectroscopy.

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장소: 제주ICC

발표코드: IV-ANAL.P-126

발표분야: 분석화학

발표종류: 포스터, 발표일시: 금 15:00~17:00

## Quantitative analysis of diquat herbicide using surface-enhanced Raman scattering-based coalescence microdroplet sensor

Rongke Gao, \*김인섭, \*최남현, \*\*주재범

한양대 응용화학과 \*한양대 바이오테크놀로지학과 \*\*한양대 생명나노공학과

Diquat (DQ) has been extensively used as herbicides in olive crops. It is toxic to algae, fish, and other aquatic organisms such as crayfish and insects. The adverse health effect of acute and chronic exposure to humans is well documented. Some countries, such as USA and Canada, make the standard for it. DQ has severe toxic effects on the central nervous system and produces lung damage even when it is not concentrated. However, the cationic character of DQ makes their determination difficult. A number of analytical methods, including high-performance liquid chromatography (HPLC), gas chromatography mass spectroscopy (GC-MS), voltammetric, and capillary electrophoresis (CE) methods, have been reported. In this work, a rapid and highly sensitive trace analysis of DQ using surface-enhanced Raman scattering (SERS)-based novel optofluidic sensor has been developed. Here, a new coalescence microdroplet channel has been fabricated for its quantitative analysis. Under the optimal condition of flow velocity, DQ molecules were effectively adsorbed onto silver nanoparticles in the channel. A quantitative analysis of DQ was performed based on the characteristic peak height in its SERS spectrum corresponding to a series of DQ concentration. According to our knowledge, it's the first time to report this new conceptual detection technology, using a SERS coalescence microdroplet sensor, for the highly sensitive trace analysis of DQ in water.

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장소: 제주ICC

발표코드: IV-ANAL.P-127

발표분야: 분석화학

발표종류: 포스터, 발표일시: 금 15:00~17:00

## Mass spectrometric Characterization of N-linked Oligosaccharides through Endoglycosidase-catalyzed Transglycosylation with the Artificial Acceptors

정수희, 임재민, \*Dong-ri Jin, 이용일

창원대 화학과 \*Department of Chemistry, Yanbian University, Yanji, Jilin, P. R. China

Analysis of glycosylation is one of major challenges due to diverse nature of post-translational modification of proteins. Detection of glycoproteins and glycan characterization is an essential sub-field of proteomics using high throughput techniques by mass spectrometry. We have used endo-beta-N-acetylglucosaminidase M (endo-M) through transglycosylation with the four artificial fluorescence acceptors for characterization of N-linked glycans by tandem mass spectrometry. In this study, we have optimized the enzymatic conditions of endo-M for transglycosylation with the acceptors and characterized the permethylated N-linked oligosaccharides from sialoglycopeptide (SGP) attached by the acceptors by mass spectrometry. Using enzymatic transglycosylation with the acceptors, we have also characterized 32 N-linked glycans from chick ovalbumin as validation of analytical efficiency by mass spectrometry.

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장소: 제주ICC

발표코드: IV-ANAL.P-128

발표분야: 분석화학

발표종류: 포스터, 발표일시: 금 15:00~17:00

## **A study on the determination of total arsenic and arsenic species in seaweed samples by ion chromatography coupled with inductively coupled plasma - atomic emission spectrometry**

나진수, CUI SHENG, 남상호

목포대 화학과

Chemical speciation of an element involves quantitative determination of the different chemical forms. The chemical speciation of elements has been very critical because their bioactivity and toxicity rely on the different chemical forms of elements in various samples. The quantitation of the total arsenic in seaweeds has routinely been performed. But, it has been very well known that toxicity and biological effect depend not only on the total concentration of arsenic but also on the chemical species of arsenic in sample. Of the chemical species of arsenic, inorganic arsenic  $As^{3+}$  and  $As^{5+}$  are highly toxic. Therefore, the importance on research of arsenic species has greatly increased. It is necessary to develop the analytical method of arsenic species because the oxidation states of arsenic species should not be converted into each other during sample preparation. This study has been focused on the sample preparation and the analytical method of total arsenic and inorganic arsenic in several seaweeds (laver, green laver, sea tangle and sea mustard) by ICP-AES (Inductively Coupled Plasma - Atomic Emission Spectrometer). The analytical method of arsenic species ( $As^{3+}$ ,  $As^{5+}$ , MMA and DMA) using IC (Ion Chromatography) coupled with ICP-AES was also investigated.



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장소: 제주ICC

발표코드: IV-BIO.P-129

발표분야: 생명화학

발표종류: 포스터, 발표일시: 금 15:00~17:00

## Metabotyping of pH Stress Adaptation of *Saccharomyces cerevisiae* as Monitored by 2 dimensional NMR Spectroscopy

채영기, \*강우영

세종대 화학과 \*세종대 화학

Metabolites of *Saccharomyces cerevisiae* under pH stress were analyzed and compared with those of the normal growth condition by two-dimensional NMR spectroscopy. NMR data were analyzed with the help of the metabolome database and the statistics software. At least 28 metabolites were identified for most of the samples. As the pH of the medium increased, the levels of many metabolites, for example, acetic acid, glucose, and serine were increased. However, as the pH of the medium decreased, aspartic acid, betaine, and ethanolamine were increased. These stress conditions were clearly clustered according to their pH, and separated from one another. Changes in individual metabolites varied significantly from sample to sample, but the combination of such changes could be used to distinguish different stress conditions from normal one, which could be done by PCA analysis. The analysis via H-1-C-13 HSQC spectra proved to be robust and effective in assessing and classifying global metabolic profiles of the yeast stress conditions.

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발표코드: IV-BIO.P-130

발표분야: 생명화학

발표종류: 포스터, 발표일시: 금 15:00~17:00

## **The Development of a Novel Point-of-Care System for the Ultra-Sensitive Detection of Anthrax Toxin as Bioterror Agent**

**박혜연, 문지영, 윤문영**

한양대 화학과

The treat of bioterrorism and the potential use of biological weapons against both military and civilian populations has become a major concern for governments around the world. For example, in 2001 anthrax-tainted letters resulted in several deaths, caused widespread public panic and exerted a heavy economic toll. *Bacillus anthracis* is a causative agent of anthrax. Anthrax toxins are composed of a protective antigen (PA), lethal factor (LF), and edema factor (EF), in which the PA is a central mediator for the delivery of the two enzymatic moieties LF and EF. Therefore, PA has been an attractive target for the toxin neutralization and diagnosis. Although accumulating reports have proposed several approaches to treat this toxin, high lethality and potential as a bioweapon place ultra-sensitive diagnostic system on serious demand. Since early detection of PA in anthrax toxin can reduce the risk of death from biological warfare and terrorism, early diagnostics method seen to be increased. However, most PA early diagnosis is currently based on the conventional antigen-antibody system, and has detection limits in the nano- and picomolar range. Therefore, our works provide a novel point-of-Care system (POCT) that can replace antibody to polyvalent peptide as a detection probe has been developed. Furthermore, a new peptide based diagnosis method for detecting anthrax proteins at extremely low concentration levels will be beneficial in accomplishing ultra sensitive and specific detection of diagnose anthrax infections.

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발표분야: 생명화학

발표종류: 포스터, 발표일시: 금 15:00~17:00

## Screening of probes bound to cancer marker Bcl-2 with a high affinity from a peptide library

박해철, \*Gedi Vinayakumar, \*윤문영

한양대 자연대학 화학과 \*한양대 화학과

The Bcl-2 protein is an integral membrane protein located mainly on the outer membrane of mitochondria. The protein encoded by the bcl-2 gene has a function as a blocker of cell death, its morphological equivalent "apoptosis". Bcl-2 protein is key regulators of apoptosis or programmed cell death associated in human disease including cancer. Actually, Bcl-2 protein has been found to be overexpressed in many cancer cells. Indeed, the Bcl-2 protein is produced overexpression in many cancer cells, including most 90% of colorectal adenocarcinomas, 30-60% of prostate, 70% of breast, 20% of non-small cell lung cancers, and 60% B cell-derived lymphomas, colorectal adenocarcinomas. Therefore, Bcl-2 protein has been an attractive target of the prevention and treatment for cancer diseases. Currently, there are no early diagnostic reagents available that specifically target Bcl-2 protein. Therefore, diagnostic tools that can detect Bcl-2 are required. In the present study, we have screened novel diverse peptides displaying on M13 bacteriophage that bind to Bcl-2 protein with high affinity (picomolar range) from a phage display library after five rounds of biopanning. These peptides can be used to develop novel diagnostic probes or potent inhibitors with diverse polyvalencies.

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장소: 제주ICC

발표코드: IV-BIO.P-132

발표분야: 생명화학

발표종류: 포스터, 발표일시: 금 15:00~17:00

## Recombinant Production and NMR Structural Studies of Antimicrobial Peptides, Lactophorin

김지선, 박태준, 최성섭, 정지호, 김용애

한국외국어대 화학과

Lactophorin (LPcin-I) is an antimicrobial, amphiphatic, cationic peptide with 23-amino acid residues isolated from bovine milk. Its analogous peptide, LPcin-II, lacks six N-terminal amino acids compared to LPcin-I. Interestingly, LPcin-II does not display any antimicrobial activity, whereas LPcin-I inhibits the growth of both Gram-negative and Gram-positive bacteria without exhibiting any hemolytic activity. Uniformly  $^{15}\text{N}$ -labeled LPcin peptides were prepared by the recombinant expression of fusion proteins in *E. coli* and their properties were characterized by electrospray ionization mass spectrometry (ESI-MS), Circular dichroism (CD) spectroscopy, and antimicrobial activity tests. To understand the structure-activity relationship of these two peptides, they were studied in model membrane environments by a combination of solution and solid-state NMR spectroscopy. We determined the tertiary structure of LPcin-I and LPcin-II in the presence of DPC micelles by solution NMR spectroscopy. Magnetically aligned unflipped bicelle samples were used to investigate the structure and topology of LPcin-I and LPcin-II by solid-state NMR spectroscopy.

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장소: 제주ICC

발표코드: **IV-BIO.P-133**

발표분야: 생명화학

발표종류: 포스터, 발표일시: 금 15:00~17:00

## Cell Penetrating Gene Carrier for Breast Cancer-targeted Therapy

이화정, 박인규, \*정서연

전남대 의생명과학과 \*전남대 의과대학 의생명과학과

A new drug delivery system with cell-penetrating peptide (CPP) gained greater attention in biomedical field. CPP facilitates intracellular uptake of target materials such as protein, gene, or macromolecules. Development of therapeutic molecule was greatly thwarted by poor uptake efficiency and low cellular trafficking, which might be overcome by chemical conjugation with CPP. In this study, we conjugated newly identified cellular penetrating peptide, which was found to be highly specific to breast cancer, to cationic gene carrier for achieving enhanced intracellular uptake. Tumor suppressor gene, p53, was delivered with CPP-conjugated gene carrier to breast cancer and its therapeutic efficacy was evaluated. The complex formation with plasmid DNA was performed by gel electrophoresis. Particle size and the surface charge were determined by DLS and zeta potential. The breast cancer transfection and targeting were tested with different breast cancer cell types and xenograft animal model.

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장소: 제주ICC

발표코드: IV-BIO.P-134

발표분야: 생명화학

발표종류: 포스터, 발표일시: 금 15:00~17:00

## **Synthesis and Charecterisation of Spion encapsulated Polymersome for MRI guided gene delivery**

**MUTHIAHMUTHUNARAYANA, 박인규**

전남대 의생명과학과

A SPION-based diagnostic property with accompanying therapeutics such as drugs or genes has been explored to improve their therapeutic efficacy. The positively charged SPION-loaded polymersome tethering PEG as a hydrophilic corona layer was prepared to deliver therapeutic genes to target sites, which was monitored by MRI concomitantly. SPION-loaded polymersome with plasmid DNA complex was checked by gel retardation assay. Hydrodynamic particle size was between 110 and 160nm, positive surface charge confirmed by zeta potential. The TGA studies confirmed that spion embedded polymersome shows more thermal stability. The transfection efficiency in vitro was tested by luciferase assay. The detectability of SPION in transfected cells by MRI was also checked. In vivo accumulation of polymerosome loaded spion in the tumor region was confirmed by MRI imaging and histo chemical analysis .Result indicates that the SPION-embedded supra-assembly can be applied to MR imaging guided gene therapy.

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장소: 제주ICC

발표코드: IV-BIO.P-135

발표분야: 생명화학

발표종류: 포스터, 발표일시: 금 15:00~17:00

## **Polycaprolactone/Polyethylenimine Electrospun Nanofibers Mediated delivery of Vascular Endothelial Growth Factor Plasmid for the treatment of Myocardial Infarction**

**CHE HUILIAN, \*이화정, \*MUTHIAHMUTHUNARAYANA, 박인규**

전남대 의생명과학과 \*전남대 분자의과학협동과정

Myocardial infarction (MI) remains the commonest cause of cardiac-related death throughout the world. In this study, we are presenting nanofiber mediated gene delivery for myocardial infarction. Branched polyethylenimine cross-linked via disulfide bonds (ssPEI) complexed with vascular endothelial growth factor (VEGF) were immobilized on the electrospun polycaprolactone (PCL)/ polyethylenimine (PEI) nanofibers for the local expression of VEGF angiogenic factor. We have studied whether the production of VEGF from myoblast cells adhering on the nanofibers has therapeutic potentials for myocardial infarction. In this method, non-specific adsorption of VEGF nanoparticles to the nanofibers occurred uniformly over all the surface area of nanofibers, resulting in increased transgene uptake and expression in more number of cells. Our results demonstrated that the delivery of therapeutic genes from biodegradable nanoparticles immobilized on the nanofiber represented minimal cytotoxicity to NIH/3T3 fibroblast cells and H9C2 myoblasts than branched PEI 25kDa did. According to luciferase assay, RT-PCR, this vector showed high transgene expression efficiency to reporter gene and VEGF gene. Surface-mediated delivery of DNA nanoparticles did not adversely affect cell growth and also facilitated the expression of transgene inside the cells.

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장소: 제주ICC

발표코드: IV-BIO.P-136

발표분야: 생명화학

발표종류: 포스터, 발표일시: 금 15:00~17:00

## A Microfluidic Approach for the Formation of Functional Synapses

Mahto Sanjeev Kumar, 이석우

공주대 화학과

In this work, we describe the formation of functional synapses between compartmentalized cortical neurons cultured inside 3-compartment microfluidic devices in a controlled fashion. The device has ability to direct the axons in an isolated compartment and thus, facilitates isolated axons to form functional synapses with dendrites of other neurons in an isolated microenvironment. In addition, the device allows the continuous real-time monitoring of neuronal processes and fluorescently tagged biomolecules. Using double immunostaining technique, synapses were characterized with the specified synaptic markers, i.e., MAP2/synapsin I and MAP5/synapsin I. To verify the process of synaptic transmission and the formation of functional synapses, the level of calcium in presynaptic terminals is observed after being induced action potential to neurons by depolarizing solution. The results revealed a significant increase in calcium influx into preferentially isolated presynaptic terminals of neurons whose cell bodies were depolarized by elevated levels of extracellular potassium ions in comparison to those of neurons that were not depolarized. In addition, we detected the presence of glutamatergic synapses and the confined movements of AMPAR GluR2 subunit inside synapses using single molecule imaging techniques. Thus, this microfluidic approach provides an easy, simple, cost-effective, and efficient way to develop synapses in an isolated microenvironment without the use of surface-patterning techniques. Furthermore, the device is also able to induce manipulations at synaptic junctions without using an electrical stimulation.



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## Clustered Magnetite Nanocrystals Crosslinked with PEI for Efficient siRNA Delivery

박지원, \*배기현, \*박태관

KAIST 자연과학 생명과학과 \*KAIST 생명과학과

Magnetofection has been utilized as a powerful tool to enhance gene transfection efficiency via magnetic field-enforced cellular transport processes. The accelerated accumulation of nucleic acid molecules by applying an external magnetic force enables the rapid and improved transduction efficiency. In this study, we developed magnetite nanocrystal clusters (PMNCs) crosslinked with polyethylenimine (PEI) to magnetically trigger intracellular delivery of small interfering RNA (siRNA). PMNCs were produced by crosslinked assembly of catechol-functionalized branched polyethylenimine (bPEI) around magnetite nanocrystals through an oil-in-water (O/W) emulsion and solvent evaporation method. The physical properties of PMNC were characterized by TEM, DLS, TSA, and FT-IR. Finely tuned formulation of clustered magnetite nanocrystals with controlled size and shape exhibited superior saturation of magnetization value. Magnetite nanocrystal clusters could form nano-sized polyelectrolyte complexes with negatively charged siRNA molecules, enabling efficient delivery of siRNA into cells upon exposure to an external magnetic field within a short time. This study introduces a new class of magnetic nanomaterials that can be utilized for magnetically driven intracellular siRNA delivery.

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## **siRNA-polycaprolactone conjugate micelles for dual delivery of chemical and nucleic acid drugs**

이수현, 이정유, 김지선, 조성덕, 박태관

KAIST 생명과학과

With high specificity and efficiency in target gene inhibition, small interfering RNAs (siRNAs) are promising tool for genomic therapeutics. However several cationic carriers, which have already shown their good transfection capacity in DNA delivery, were not competent in siRNA delivery because of low charge density and small size of siRNA compared to large plasmid DNA. In our previous study, biodegradable and biocompatible PLGA was conjugated to 3' end of siRNA by a disulfide bond and the resultant hydrophobic polymer-siRNA hybrid formed a micellar structure in an aqueous environment. We demonstrated that these self-assembled micelles overcame insufficient charge density and formed more compact and stable complex with cationic carrier. Here, we synthesized polycaprolactone-siRNA-PEG triblock copolymers to form a micellar structure because of their amphiphilic property. The hydrophobic polycaprolactone parts located in the core of micelles contribute to increase the siRNA charge density while the distally exposed PEG parts enhance the particle stability and protect siRNAs against enzymatic attacks. We also encapsulated hydrophobic drugs, paclitaxel, in the core of micelles for dual delivery of siRNAs and chemical drugs to problematic cells. With dual therapy of anti-apoptotic gene targeting siRNAs and anti-cancer drug, bcl-2 siRNA and paclitaxel, respectively, the enhanced cell death was observed.

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## Construction and characterization of the reconstitutable zinc finger nuclease

박소영, 김건섭, \*WEILIJIE, \*ZHENGXU, 김양균

성균관대 화학과 \*성균관대 화학학과

Zinc finger nucleases (ZFNs) are artificial restriction enzymes consisted of modular structure of C2H2-type zinc finger domains and the FokI nuclease domain (FN). Typically, ZFNs can be created by fusing multiple zinc fingers (for DNA recognition) to the FN domain (for DNA cleavage). Recently, ZFN technology received much attention because it is envisioned as a powerful tool for genome engineering. For wider use of the rapidly progressed ZFN technology, it is required to overcome many technical obstacles. In this study, we aim to develop a rapid and facile screening and assay system for producing reliable ZFNs that possess high sequence-specific recognition and cleavage activities. In our strategy, complete ZFNs are non-covalently reassembled from separately expressed zinc finger domain and FN that fused to one of anti-parallel leucine zippers, respectively. Our result showed that these reconstitutable ZFNs (reZFN) assembled through the formation of anti-parallel dimeric leucine zippers successfully cleaved target sites in a sequence-specific manner. Thus, our result establishes a novel screening system based on mix-and-match strategy to examine binding and cleavage of ZFNs against target DNA sequences. In the future, our work will contribute to creating optimized ZFN technology to apply in various applications such as gene manipulation and gene therapy. 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 (2009-0075300).

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## **siRNA Hydrogel Microparticles for Gene Silencing**

홍철암, 이수현, 김지선, 박지원, 배기현, 박태관

KAIST 생명과학과

Nucleic acids, DNA and RNA, have been exploited as excellent molecular building blocks for fabricating a wide range of two- and three-dimensional nanostructures with different sizes, shapes, and patterns due to its highly selective base pairing ability between the complementary sequences. A variety of predictable nanoarchitectures including grids, cubes and polyhedra could be readily constructed in a precisely controlled manner by rationally designing an array of self-assembling DNA molecules. DNA based dendrimers and hydrogels were also synthesized by using Y-shaped DNA molecules that serve as crosslinkers for self-assembling two or more combinatorially designed sequences. Although the self-assembled DNA nanostructures and hydrogels exhibit hierarchical and supramolecular structures in a well-defined geometry, they generally do not show any biological activities in a molecular and cellular level. Small interfering RNA (siRNA), double-stranded (ds) RNA molecules with 21 ~ 27 base pairs, has recently emerged as a powerful tool for silencing a target gene. Compared to single-stranded (ss) antisense oligonucleotides, siRNA has shown more efficient gene silencing with higher specificity and lower doses. In this study, we demonstrated a novel strategy to prepare biologically active siRNA-based hydrogel structures through self-assembly process between complementary ss sense and antisense siRNA species using Y-shaped siRNA as crosslinkers. The siRNA-based microgels with substantially increased charge density were drastically collapsed to form compact nano-sized complexes upon interacting with a less charged cationic polymer carrier, and the complexes exhibited superb cellular uptake and gene silencing activities.

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## Development of gold-iron oxide nanoparticle probe for dual diagnosis

문명주, \*이화정, 볼로르마, HANSHANHUA, \*박인규, 정용연

전남대 영상의학과 \*전남대 의생명과학과

Nowadays, diagnosed cancer by using CT(Computed Tomography) and MRI(Magnetic Resonance Image) are widely popular however, each of them has got some disadvantages. In order to cross over their problems and give exact diagnosed result, CT and MRI are combined together. Respectively, gold and iron oxide were used as the contrast agent for cancer diagnosis by CT and MRI. Therefore, it will be perfectly when one probe was synthesized for both diagnosis. Here, multi-imaging nanoparticle that consist of gold and iron oxide were synthesized. Sense and anti-sense oligodeoxynucleotide (ODNs) were used in order to link the iron and gold particles together when they are hybridized. For enhancing haft life of the particles, their surface was coated with poly ethylene glycol (PEG). Physicochemical properties of multi-imaging nanoparticles were characterized by TEM, DLS, Zeta-potential. As the result, gold and iron oxide particles were stably linked to each other due to the hybridization of ODN. Also, the sizes of particle can be adjusted by controlling the amount of ODN on their surface. Lately, the particles were showed their detectable in CT and MRI.

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## **Quantum Dot Core Cationic Solid Lipid Nanoparticles for Synergistic Paclitaxel-siRNA Combination Therapy and Fluorescent Cancer Detection**

배기현, 이정유, 이수현, 도민재, 박태관

KAIST 생명과학과

Small interfering RNA (siRNA) has recently emerged as a promising therapeutic agent for cancer treatment due to its superior ability to silence target genes specifically. Herein we report the development of cationic solid lipid nanoparticles incorporating quantum dot nanocrystals as a multifunctional carrier for paclitaxel-siRNA combination therapy and fluorescent cancer detection. These nanoparticles could stably encapsulate paclitaxel in their interior and also form nanosized polyelectrolyte complexes with siRNA molecules. We found that they efficiently delivered paclitaxel and anti-cancer siRNA into human lung cancer cells, and thus induced apoptotic death of the cancer cells in a synergistic manner. Moreover, the intrinsic fluorescent property of the incorporated quantum dots enabled simultaneous visualization of the cancer cells with a conventional optical imaging device.

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## **Synthesis and characterization of Dual sensitive(Temperature and pH) polymers Based on Polycaprolactone.**

남정아, 김인식, 박성영

충주대 화공생물공학과

We prepared double stimuli responsive PCL-g-(NIPAAm-co-DEA) and mPEG-PCL-g-(NIPAAm-co-DEA) micelles that responded to change in temperature and pH. During synthesis we used the thermoresponsive polymer NIPAAm having an LCST of 32°C and a pH sensitive polymer 2-(diethylamino) ethyl methacrylate (DEA). Because of this two polymers, our finally synthesized polymers show temperature and pH responsiveness when they are subjected against these stimuli. The chemical structure was confirmed by <sup>1</sup>H NMR and FT-IR instruments. The dual responsiveness of the polymers was investigated via dynamic water contact angles and the results showed that the contact angles were increased by increasing pH. The pH-dependent LCST was confirmed by cloud-point. The mPEG-PCL-g-(NIPAAm-co-DEA) and PCL-g-(NIPAAm-co-DEA) with thermal- and pH-sensitive properties can be applied as controlled release carriers for biomedical applications.

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## **Study of Interaction Between Influenza NS1 Protein and DNA Aptamer**

우혜민

국민대 화학과

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 inhibits the host innate immune responses during viral infection, so that interferon (IFN) is prevented. In this study, DNA aptamers against NS1 protein were isolated from DNA library containing random sequences of 40 nucleotides using a SELEX (systematic evolution of ligand by exponential enrichment) procedure. After 15 rounds of selection, DNA aptamers that specifically bind to the NS1 protein were isolated and shown to have different binding capacities. And we investigated the interaction between NS1 protein and aptamers by Sandwich ELISA and EMSA.



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## **In Vitro Selection of DNA Aptamers against Spike Protein of SARS Coronavirus**

우혜민

국민대 화학과

The spike protein (S) of Severe Acute Respiratory Syndrome (SARS)-CoV mediates infection of receptor-expressing host cell. It is believed that S protein is one of the most promising antigen candidates for vaccine design of a newly emerged disease SARS. In this study, DNA aptamers against S protein were isolated from DNA library containing random sequences of 40 nucleotides using a SELEX (systematic evolution of ligand by exponential enrichment) procedure. And we investigated the interaction of S protein with aptamers by Sandwich ELISA and EMSA. The aptamers that were isolated in this study are expected to be new molecular probes as well as therapeutics for the design of SARS-Co V diagnosis and treatment.

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## Application of Multi Sensitive Crosslinked Pluronic Micelles as a Carrier to Deliver Anti Cancer Drug Paclitaxel

NAHAIN ABDULLAH AL, 박성영

충주대 화공생물공학과

Multi sensitive crosslinked Pluronic F 127 micelles have been designed to deliver hydrophobic anticancer drug paclitaxel. Dynamic laser light scattering (DLS) investigation was performed to measure the micelle size which indicates that the hydrodynamic diameter of the formed empty micelles was  $38.6 \pm 10.9$  nm wherein it was  $99.5 \pm 26.2$  nm after paclitaxel loading. The morphology of the micelle was evaluated through transmission electron microscopy (TEM). By using quantum dots, the stability of the micelles was examined under different reductive conditions (by using dithiothreitol as reductive agent) and acidic environment. Stability of the micelles was found at pH 7.4 but the micelles were not stable at lower pH and higher reductive environment. By using the hydrophobic drug paclitaxel we measured the drug release profile. The drug loading efficiency was 33.4% and 85% drug was released when the micelles were subjected at pH 5.0 after 72 hours and complete drug release was found in higher reductive environment ( in 70 mM DTT). Using A549 human lung cancer cells, toxicity of the synthesized micelles and paclitaxel loaded micelles were performed with MTT assay. 100% cells were viable up to higher concentration of the polymer (2mg/ml) indicating that the synthesized polymers are not toxic. Only 25% cells were viable when the micelles contain 1  $\mu$ g/ml paclitaxel in the micelles. The cellular uptake of the paclitaxel-loaded micelles was investigated in more detail by confocal microscopy.

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## Synthesis and Characterization of Thermo / pH sensitive hydrogel based on Pluronic

오연정, 박성영

충주대 화학생명공학과

New hydrogels exhibiting pH and temperature triggered drug release capability have been synthesized by grafting thermosensitive moiety poly(N-isopropylacrylamide) and poly(N,N-Diethylaminoethyl methacrylate) and poly(methacrylic acid) as pH sensitive moieties by modifying Pluronic F-127 (poly(ethylene glycol) (PEO-PPO-PEO)). Characterization of these two polymers was evaluated via <sup>1</sup>H NMR investigation. The LCST of both polymers were investigated under different pH. The results showed that at lower pH the LCST of the Pluronic-NIPAAm-DEAEMA was increased due to protonation of DEAEMA. At higher pH, LCST of Pluronic-NIPAAm-MAAc was increased as in this pH carboxyl (-COOH) are ionized. We investigated the contact angles and DLS experiments for both polymers where both of the polymers showed significant changes in their behaviors when they were subjected against lower and higher pH individually due to ionization. Finally rheological behavior of these polymers were examined where the results indicate that the moduli of the hydrogels were able to be tuned with chemical composition against pH and temperature. The findings from all experiments support to show that the synthesized Pluronic-NIPAAm-DEAEMA and Pluronic-NIPAAm-MAAc copolymers can be expected to behave as temperature/pH-sensitive polymers exhibiting a sol-gel transition under physiological conditions are useful for diverse biomedical applications such as delivery of bioactive macromolecules, tissue engineering, and drug-delivery systems.

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## Engineering of IF-insertion hybrids, FKBPIF and F36VIF

신은숙, \*이경희

세종대 화학과 생화학 \*세종대 화학과

We aim to investigate the role of molecular chaperones which can regulate some specific proteins (such as IAPP or Syn) aggregating into fibrillar structures under pathological conditions. In order to obtain more powerful chaperones than FKBP12, we have designed the FKBPIF and F36VIF hybrids, which were engineered as insertion hybrids of IF (insertion-in-flap) domain into FKBP12 and F36V genes, respectively. Using PCR and site directed mutagenesis, these FKBP hybrid genes (FKBP, FKBPIF, F36V and F36VIF) were sequentially cloned in the pET28-based system to contain N-terminal His6 tags for further purification. Upon induction with 0.5mM IPTG, FKBP hybrid proteins were successfully expressed and purified by Ni<sup>2+</sup>-column affinity chromatography in one step. The in vitro biochemical characteristics of these hybrid proteins are also examined in point of molecular chaperones and PPIase (peptidyl-prolyl cis-trans isomerase) activities.

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## **Traceless immobilization of proteins using naturally split Npu. DnaE intein mediated protein trans-splicing.**

민경미, 정덕호, 권영은

동국대 의생명공학과

Biochips provide useful platforms for various biological assays. Especially, protein chips make useful tools for screening protein-protein interaction and characterizing the level of proteins expressed in cells. The fabrication of protein chips requires immobilization of probe proteins onto a solid support. Current strategies for protein immobilization include non-covalent adsorption of proteins, covalent cross-linking of proteins and affinity-tag based immobilization of proteins. These immobilization strategies often suffer from several limitations such as non-specific adsorption of proteins, loss of protein activity due to denaturation and false positive results mediated by linker proteins. Incompatibility with quantitative analysis and lack of reproducibility are often problematic, as well. In this work, we are developing an approach for effective immobilization of proteins using naturally split Npu. DnaE intein mediated protein trans-splicing. In this approach, C-terminal fragment of split-intein is chemically introduced to the solid substrate and target proteins fused to the N-terminal fragment of intein is immobilized through trans-splicing reaction. By immobilizing proteins of interest through specific interaction of peptide fragments, proteins can be selectively attached to the chip surface with a uniform orientation without the presence of linker proteins. This controlled immobilization result in functional protein chips that can be used for quantitative analysis of crude biological samples. Authors gratefully acknowledge the financial support from the Korea Ministry of Education, Science and Technology by Basic Science Research Program through NRF (Grant No. 20100028054) and the Korea Food & Drug Administration (Grant No. 10182KFDA 991) in 2011

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## Measurement of cellular migration rate upon treatment with small molecules SG12 & SG14

정덕호, 민경미, 권영은

동국대 의생명공학과

Cell migration is an essential process for survival and differentiation of cells. A number of diseases are induced or influenced by inappropriate regulation of cellular migration. Especially, cellular migration is a well-known mechanism for cancer cell metastasis and it is important to understand the factors that affect cell migration for effective treatment of cancers. In this work, we have investigated the effect of newly identified sphingosine kinase (SphK) inhibitors (SG12 and SG14) on cellular migration. The tested SG12 and SG14 are synthetic analogs of sphingoid, a natural inhibitor of SphK, and known to specifically inhibit the functions of SphK2. Three different cell types (HeLa, HER2, and 3T3) were tested and inhibition of cellular migration was observed in all cases but with different extend. Both molecules (SG12 and SG14) showed more efficient inhibition compared to control batches treated with known inhibitor, N,N-dimethylsphingosine (DMS). The retarded migration was also more pronouncing with cancerous cell lines (HeLa, HER2). This observation was further invested by monitoring the changes in expression levels of motility-related proteins upon exposure to the test molecules. Authors gratefully acknowledge the financial support from the Korea Ministry of Environment (Grant No. 212-101-003 and 091-091-089) and the Korea Ministry of Education, Science and Technology (Grant No. 20100010553, Basic Research Program).

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## Real-time detection of caspase activity

강효진, \*정상전

과학기술연합대학원대 나노바이오 공학 \*한국생명공학연구원 바이오나노연구단

Based on FRET technology and intrinsic protein fluorescence, we have developed highly sensitive, real-time detectable and label-free detection method (intrinsic FRET; IFRET). Unlike conventional FRET requiring target-labeling with fluorescence molecules, IFRET does not require artificial fluorescence labeling step thereby conserving inherent function of target proteins during the experiment. We observed IFRET signal from the active caspase-3 with its specific IFRET probe. Due to proximity of the probe to fluorescent amino acids in the target protein as well as high quantum yield of the probe, the apparent FRET efficiency was observed more than 100% in our measurement in vitro. Whereas, the probe was exposed to catalytically mutated caspase-3, it did not show a meaningful FRET signal, meaning that the high FRET efficiency comes from specific binding of the probe to the active site of caspase-3. This technique will be useful for tracking proteins of biological importance in cells, for developing a high throughput screening system (HTS) of drugs, and real-time enzyme.

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## Human protein tyrosine phosphatases (PTPs) as potential tools for phosphoprotein analysis

정명선, 강효진, \*이영미, \*\*정상전

과학기술연합대학원대 나노바이오공학 \*한국생명공학연구원 바이오나노연구단 \*\*한국생명공학연구원 바이오나노연구단

Phosphorylation-dephosphorylation on protein tyrosines, which is balanced by relative activities of PTKs (protein tyrosine kinases) and PTPs (protein tyrosine phosphatases), serves as a crucial tool to regulate important cellular signal transduction controlling the shape and motility of cells, cell proliferation, organ development, and immune system. Interference of this balance, therefore, has been implicated in various diseases such as cancers, inflammation, and immune deficiencies. Human body has at least 107 PTPs of which physiological roles remain to be fully identified. Since PTPs bind to phosphoproteins as substrates, they may offer attractive tools, such as affinity column for phosphoproteins, phosphoprotein-modulators etc, to analyze phosphoproteins. In order to test their utility to study phosphoproteins in proteomics level, we have cloned, expressed by using E. coli expression system, and purified over 70 human PTPs, and their mutants to facilitate stronger binding to the substrates and better cell permeability. In this conference, we will introduce the cloning, expression, and purification of human PTPs described above and our effort for their biochemical applications.



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## Synthetic peptides as a platform for immunohip surface and Ab purification

이영미, \*강효진, \*\*정상전

한국생명공학연구원 바이오나노연구단 \*과학기술연합대학원대 나노바이오공학 \*\*한국생명공학연구원 바이오나노연구단

Antibody immobilization on a solid surface is an inevitable process in the preparation of immunohips/sensors. Previously, we described a novel strategy to immobilize an antibody on various sensor surfaces by using small cyclic peptides which bind to IgG Fc domain in a specific manner. SPR analysis indicated that a peptide linked to a gold chip surface through a hydrophilic linker efficiently captured human IgG with strong binding affinity ( $K_d = 85$  nM) to human IgG, comparable to that of monomeric Protein G ( $K_d = 110$  nM). In addition, the FcBP peptide was immobilized on sepharose resin to prepare affinity columns for antibody purification and compared its Ab-binding capacity with those of Protein A and G columns. The results demonstrated that FcBP column has a similar purification ability of IgG to the protein columns but showed improved stability in cleaning in place (CIP) steps, affording almost constant purification stability for 30 runs in spite of repetitive acid/base washing. This, together with the chip application described above, demonstrates that FcBP is a viable immunological platform for Ab purification and immunohip technology.

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## Small Angle X-ray Scattering Studies on Structures of Biological Molecules in Solution

진경식, \*이문호

포항공과대 포항가속기연구소 \*포항공과대 화학과

The fundamental aim of structural studies in molecular biology is to establish a relationship between the structure (or, more precisely, structural changes) and function of biological macromolecules. Over the past years, a tremendous amount of structural information has been obtained using macromolecular crystallography and nuclear magnetic resonance (NMR). These high-resolution methods apply only in rather specific conditions: it is often difficult to grow crystals of high molecular weight (MW) assemblies that are suitable for diffraction, and the application of NMR is fundamentally limited to small (MW < 30 kd) proteins. Investigation of structure of biological macromolecules in solution remains one of the most important fields of application of small angle X-ray scattering (SAXS) technique. SAXS permits analysis of biological macromolecules and their complexes in nearly physiological environments and direct study of structural responses to changes in physical and chemical conditions. Recent remarkable progress in instrumentation, in particular thanks to high-flux dedicated X-ray synchrotron radiation has significantly improved the quality of the experimental SAXS data. This method is an important complementary tool to the high-resolution techniques (X-ray crystallography and NMR). The fundamental aim of this study is to obtain more detailed information on the structure and structural differences of a variety of biological macromolecules in solution under various conditions by using SAXS technique. Ultimately, the structural evidence presented here will contribute to a better understanding of relationship between structures of macromolecules and their function, from a biophysics point of view.

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## A novel chroman derivative induces apoptosis in human cervical carcinoma HeLa cell in response to DNA damage

Zhangxin, 황지영, 이명진, \*신동수, 김동규

인제대 화학과 \*창원대 화학과

In this study, 1-((3S,4R)-4-(2-Ethoxy-4-methyl-1H-pyrrol-1-yl)-3-hydroxy-2,2-dimethylchroman-6-yl)-3-phenylurea (S24), a novel 4,6-disubstituted 2,2-dimethylchroman was synthesized and its anticancer activity was investigated on the in vitro growth of human cervical carcinoma HeLa cells. In this study, we showed that S24 inhibited HeLa cell proliferation and viability in dose-dependent and time-dependent manner and the IC<sub>50</sub> value was about 150  $\mu$ M. DNA damage after S24 treatment was observed as early as 12 hr in the very sensitive alkaline microgel electrophoresis technique (comet assay). [<sup>3</sup>H]thymidine incorporation and flow cytometry analysis revealed that S110 treatment significantly inhibited DNA synthesis and arrested HeLa cells at the G0/G1phase of the cell cycle after 24hr. The cells exhibited apoptotic morphology like condensed chromatin and nuclear fragmentation after 48 hr of treatment. Furthermore, the results from Annexin V-FITC/PI dual staining indicated that S24 induced early apoptosis in HeLa cells after exposure to S24 for 48hr. We also found that treatment of cells with S24 significantly increased the levels of the pro-apoptotic protein Bax, which is regulated by p53, suggesting the possible involvement of interaction between S24 and p53 regulated apoptotic pathway. Subsequently, caspase activation involving caspase-9 and -3 by western blot analysis was observed. These findings suggest that S24 induces HeLa cell apoptosis by caspase-dependent intrinsic apoptotic pathway in response to DNA damage.

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## **A novel chroman derivative causes DNA damage and triggers apoptosis via caspase- and mitochondria-dependent pathways in human cervical carcinoma HeLa cell**

**Zhangxin, 황지영, 이명진, \*신동수, 김동규**

인제대 화학과 \*창원대 화학과

(3R,4S)-2,2-dimethyl-6-nitro-4-(4-(3-(trifluoromethyl)phenyl)piperazin-1-yl)chroman-3-ol (S110), a novel 4,6-disubstituted 2,2-dimethylchroman was synthesized and its anticancer activity was investigated on the in vitro growth of human cervical carcinoma HeLa cells. In this study, we showed that S110 inhibited HeLa cell proliferation and viability in dose-dependent and time-dependent manner and the IC<sub>50</sub> value was about 17  $\mu$ M. DNA damage after S110 treatment was observed as early as 12 hr in the very sensitive alkaline microgel electrophoresis technique (comet assay). [<sup>3</sup>H]thymidine incorporation and flow cytometry analysis revealed that S110 treatment significantly inhibited DNA synthesis and arrested HeLa cells at the G0/G1phase of the cell cycle after 24hr. The cells exhibited apoptotic morphology like condensed chromatin and nuclear fragmentation after 24 hr of treatment. Furthermore, the results from Annexin V-FITC/PI dual staining indicated that S110 induced early apoptosis in HeLa cells in time-dependent manner after exposure to S110 for 24hr. Western blot analysis showed increase in levels of mitochondrial apoptogenic factors Bax, cytochrome-c followed by activation of caspases-9 and -3 leading to apoptosis. Results of this study showed that the anticancer activity of S110 is the underlying mechanism by which S110 causes DNA damage and apoptosis via caspase- and mitochondria-dependent pathways.

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## **Reducible dextran-siRNA conjugates for efficient gene silencing**

김지선, 박재윤, 박태관

KAIST 생명과학과

Small interfering RNA has been considered as one of the most promising therapeutics for treating various diseases such as cancer and infections as well as genetic diseases. However, siRNA has different physical characteristics from plasmid DNA due to its short persistent length and low charge density, making it difficult to complex with low molecular weight cationic polymers and lipids. Thus, a wide array of cationic and reducible carriers such as polymers, lipids, peptides and micelles are exploited to form stable siRNA nano-complexes or siRNA structure was modified to produce multimeric siRNA, PEG conjugated siRNA and siRNA conjugate micelle structures. Here, we propose a new class of siRNA polymer conjugates using neutral dextran. As proved in the previous paper, multimeric siRNA with higher cationic charge density and increased flexibility could easily form compact polyplexes and be delivered into the cell effectively. Similarly, dextran conjugated multiple siRNAs are hypothesized to show highly efficient gene silencing behaviors by forming stable polyplexes with cationic polymers.

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## **High-throughput screening assay of SARS-CoV helicase inhibitors.**

유미선, 이진무

국민대 화학과

Severe acute respiratory syndrome(SARS) is a respiratory disease which is caused by the SARS coronavirus(SARS-CoV). SARS spread from the Guangdong province of China and has a case-fatality rate of 9.6%. (According to the WHO, 21 April 2004) SARS-CoV helicase is a requisite for virus replication. So we select the SARS-CoV helicase as a target for anti-SARS therapy. We purified this protein by Ni-chelated affinity chromatography and Sephadex G-100 gel-filtration column chromatography. High-throughput screening(HTS) assay is used to find out inhibitors of SARS-CoV helicase. HTS assay is carried out 2 parts for confirming activity of helicase. First part is FRET-based duplex DNA unwinding activity test and second part is ATP hydrolysis activity test. The compound YC102 had an IC<sub>50</sub> value of  $10.9761 \pm 0.2949 \mu\text{M}$  for SARS-CoV Helicase duplex DNA unwinding. The compounds YC99 and YC102 had IC<sub>50</sub> values of  $9.5030 \pm 0.2348 \mu\text{M}$  and  $3.9072 \pm 0.0440 \mu\text{M}$  for SARS-CoV Helicase ATP hydrolysis, respectively. We expect that the YC compounds will be useful in vitro for the development of antiviral agent against SARS-CoV.

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## **Poly( $\gamma$ -glutamic acid) Nanogels for Drug Delivery Applications**

배희호, 임용택

충남대 분석과학기술대학원 분석과학기술학과

In this study, we have made poly( $\gamma$ -glutamic acid) ( $\gamma$ -PGA) based nanogels cross-linked with disulfide linkages for drug delivery applications. The  $\gamma$ -PGA nanogels were synthesized by forming nanocomplexes with thiolated  $\gamma$ -PGA, poly(ethylene glycol) (PEG), and doxorubicin (DOX) as a model drug in a selected organic solvent. Intermolecular disulfide bonds were generated between thiol groups (-SH) of thiolated  $\gamma$ -PGA molecules by ultra-sonication. The average size of  $\gamma$ -PGA nanogel was  $105.4 \pm 30.7$  nm in aqueous solution. DOX-loaded  $\gamma$ -PGA nanogels had a great effect on cell death, while the nanogels without DOX didn't seriously affect on cell viability. Moreover, DOX-loaded nanogels have shown better cell uptake than free DOX, that was confirmed by FACS analysis. Anticancer drugs were controlled released from the disulfide cross-linked  $\gamma$ -PGA nanogels by reducing agent such as glutathione (GSH) or dithiothreitol (DTT). The present study suggests that biocompatible and biodegradable  $\gamma$ -PGA based nanogels can be used as a smart drug delivery carrier.

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## **Nanoparticles for MR/Activatable Fluorescence Multi-modality Biomedical Imaging of Cancer Cells**

이지연, 김현민, 임용택

충남대 분석과학기술대학원 분석과학기술학과

Here, we have fabricated nanoparticles containing both superparamagnetic iron oxide nanoparticle and pH activatable fluorescent probe for multi-modality MR/optical imaging. We present a multi-modality imaging technologies to image live cells using pH activatable fluorescent probe coated Mn-SPIO nanocomposites. The antibody conjugated multi-modal imaging nanoprobe were efficiently delivered in live SKBR3 breast cancer cells and imaged through both MRI and optical imaging techniques. The multi-modality nanoprobe are expected to be used in the diagnosis of viable cancer cells and trafficking of therapeutic cells.



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## Electrostatically Self-assembled Hybrid Nanoparticles for High Performance MRI Contrast Agents

김현민, 임용택

충남대 분석과학기술대학원 분석과학기술학과

Manganese-doped superparamagnetic iron oxide nanoparticles ( $\text{MnFe}_2\text{O}_4$ ) were efficiently encapsulated with biocompatible polyelectrolytes by ionic assembly between poly- $\gamma$ -glutamic acid ( $\gamma$ -PGA) and poly-L-lysine (PLL).  $\text{MnFe}_2\text{O}_4$  synthesized via thermal decomposition method in organic phase were ligand-exchanged with  $\gamma$ -PGA for the transfer into aqueous phase.  $\text{MnFe}_2\text{O}_4$  coated with negatively charged  $\gamma$ -PGA were assembled with a cationic polymer, PLL, through electrostatic interaction, resulting in polymer based nanoparticles containing a cluster of  $\text{MnFe}_2\text{O}_4$ , PLL/ $\gamma$ -PGA/ $\text{MnFe}_2\text{O}_4$  (LPM). Then, LPM NPs were PEGylated for the stability in a wide range of pH. The structure and morphology of PEG-LPM NPs were determined by SEM, TEM and DLS. PEG-LPM NPs displayed high value of MRI relaxivity ( $r_2$ ), 436.8 (Mn+Fe)  $\text{mM}^{-1}\text{s}^{-1}$ , which is much higher than those of conventional iron oxide-based and  $\text{MnFe}_2\text{O}_4$  based MRI contrast agents, due to their synergic magnetism effect. PEG-LPM NPs were easily taken up into the cancer cell and showed a strong darkening effect in  $T_2$ -based MR images.

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## **Multifunctional siRNA delivery system using streptavidin-biotin interaction**

조성덕, 이수현, 박태관

KAIST 생명과학과

Small interfering RNA (siRNA) of 21 base pair can suppress a target gene selectively at the mRNA level by a process called RNA interference (RNAi). Synthetic siRNA has considered a new class of nucleic acid drug for treatment of various diseases, including viral infection and cancer. Despite the high therapeutic potential of siRNA, safe and efficient delivery problems are major hurdles to clinical applications. In our previous study, multimeric siRNA chemically crosslinked produced more stable polyelectrolyte complex with less toxic carriers and showed enhanced gene silencing efficiency because of increased charge densities and flexibilities. Here, we introduced streptavidin molecules into the multimeric siRNAs to incorporate various functionalities. We expect that the system can be easily modified with a variety of biotin containing molecules for targeting and imaging.

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## **An alternative to Western blot analysis using RNA aptamer-functionalized quantum dots**

신선미, 김일현

경희대 화학과

To make full use both of optical properties of quantum dots (QDs) and of specific interactions between aptamers and their ligands of interest, we employed QD-conjugated RNA aptamer interactions with histidine tag. QDs offer revolutionary fluorescence performance due to their long-term photostability, brilliant colors, fixability, and narrow, symmetrical emission spectra, and aptamers are known to specifically bind to their target molecules, including metal ions, small molecules, and macromolecules. In this study, we have synthesized RNA aptamer-functionalized QDs, and demonstrated their application to specific protein detection, as an alternative to the conventional Western blot analysis. We observed that our RNA aptamer-functionalized QD system dramatically reduced the time and effort required for conventional Western blot analysis, whereas the selectivity was comparable to that of the conventionally available anti-histidine tag antibody and the sensitivity was comparable to that of the Coomassie blue staining method. In principle, owing to the remarkable optical properties of QDs and a wide versatility of aptamers for selection, our system can harness the high brightness, stability and reusability to quantitatively detect aptamer-recognizable proteins. Furthermore, multiplex detection for several proteins on a single blot can be achieved by our new method, which thus may be able to facilitate and simplify the routinely used protein detection procedure, and make a variety of proteomics analysis possible.

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## Functionalized quantum dots to quantify NADPH and their use for NADP<sup>+</sup>-dependent biocatalyzed transformations

김예슬

경희대 화학과

Quantum dots are semiconducting nanoparticles that can be prepared with interesting optical properties. The fluorescent properties of quantum dots are one of the key advantages for their use as optical labels for biorecognition events and biocatalytic processes. We have prepared semiconductor quantum dots conjugated with Nile Blue (NB), and demonstrate that NB-functionalized quantum dots can act as versatile probes to analyze different biocatalyzed transformations, and can be used for the quantitative detection of NADPH as well as NADH. This approach provides a new path for the optical detection of NAD(P)H and for the quantitative analysis of NAD(P)<sup>+</sup>-dependent biotransformations.

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## Fabrication of a Structure-Specific RNA Binder for Array Detection of Label-Free MicroRNA

이정민, \*정용원

과학기술연합대학원대 나노바이오공학과 \*한국생명공학연구원 바이오나노연구단

Monitoring expression patterns of microRNAs (miRNAs) has become critical for the study of gene expression regulation. Moreover, miRNA profiling shows great potential for clinical applications such as diagnosis and evaluation of drug efficacy. Well-established DNA microarray detection tools have been widely applied for miRNA profiling. These methods, however, require miRNA labeling processes, which generally utilize direct or indirect enzymatic (or chemical) labeling reactions against target miRNAs prior to (or sometimes after) hybridization to chip surface probes. This process would be greatly simplified by the development of a miRNA array detection method a) free from labeling reactions, b) without amplification steps, and c) utilizing well-established DNA microarray platforms. These improvements would clearly bolster the credibility of miRNA profiling studies, particularly in the realm of diagnostics. In the present work, we introduce the first example of a binding-protein based array detection of miRNA. We fabricated a novel structure-specific RNA binding protein by blending native RNA binding motifs. The fabricated protein conjugate stably (slow dissociation) and specifically ( $K_d = \sim 7.3$  nM) binds to double-stranded RNAs with a 2-nucleotide 3' overhang. Acting like an antibody, this RNA binder allows universal detection of hybridized miRNAs on array surfaces without any enzymatic amplification or labeling reactions. This work presents the design and construction of the structure-specific RNA binding protein, RNA-binding characteristics of the conjugate, and the successful applications for fluorescence microarray detection of human miRNAs.

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## **Two-step synthesis of 50-deoxy-50-thioguanosine-50-monophosphorothioate and its incorporation efficiency into 50-terminus of RNA for preparation of thiol-functionalized RNA**

김일현, 신선미

경희대 화학과

Several 50-modifications of RNA molecules have been shown to have broad applications in studying RNA structures, mapping RNA-protein interactions, and in vitro selection of catalytic RNAs. While phosphorothioate modification is one of the most popular methods for functionalizing the 50-terminus of RNA by a transcription or kinase reaction, conjugation of terminal phosphorothioates with fluorophores has been achieved only with a low efficiency. To overcome this limitation, we have developed a two-step synthetic method for 50-deoxy-50-thioguanosine-50-monophosphorothioate by combining two known reactions and measured its incorporation efficiency into the 50-terminus of RNA by in vitro transcription using T7 RNA polymerase that requires guanosine to efficiently initiate transcription, followed by treatment of alkaline phosphatase, yielding a terminal sulfhydryl group at the 50-termini of RNA molecules. Since the sulfhydryl group can be used as an alternative to phosphorothioates, our method may provide a useful route to efficiently introduce reporters, such as fluorophores, into the 50-terminus of RNA via a stable thio-linker, or to tether the oligomer to a solid support.

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## Non-linear pharmacokinetic of PDE-310, a novel PDE 4 inhibitor

송진숙

충남대 약학대학

A novel phosphodiesterase-4 inhibitor, 2-aryl-7(3',4'-dialkoxyphenyl)-pyrazolo[1,5- $\alpha$ ] pyrimidine (PDE-310), has been synthesized for the treatment of respiratory diseases. We evaluated PDE-310 with respect to its pharmacokinetics and tissue distribution in rats, as well as microsomal stability, Caco-2 cell permeability, plasma protein binding, and cytochrome P450 inhibition. High liver microsomal stability of PDE-310 in humans and rats suggested a low first-pass effect and high bioavailability. PDE-310 exhibited high Caco-2 cell permeability in the absorptive direction (apparent permeability coefficients,  $\sim 20 \times 10^{-6}$  cm/s), with higher transport in the secretory direction, giving efflux ratios of 3.9 and 2.6 at 5 and 10  $\mu$ M, respectively. However, high efflux ratio and improved absorption by the treatment of efflux transporter inhibitors indicate their involvement in the intestinal transport. PDE-310 bound strongly to human plasma proteins, whereas significantly more PDE-310 (27-34%) was free in rat plasma. Following intravenous administration, non linear elimination of PDE-310 was observed at the tested dose ranges ( $K_m$ , 0.22 mg/L;  $V_{max}$ , 127.3 mg $\cdot$ hr $^{-1}$  $\cdot$ kg $^{-1}$ ). Following oral PDE-310 administration, dose-normalized AUC and  $T_{max}$  increased significantly in a dose-dependent manner. Thus, PDE-310 has a non-linear pharmacokinetic characteristics and good oral bioavailability, mediated by high metabolic stability and intestinal cell permeability, and slow absorption, owing to prolonged gastric retention and active efflux transporters.

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## Molecular Basis for the Enantioselective Hydrolysis of $\beta$ -Substituted- $\gamma$ -acetyloxymethyl- $\gamma$ -butyrolactones by *Burkholderia cepacia* Lipase

엄희성, 하현준, \*이원구

한국의국어대 화학과 \*서강대 화학과

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. Furthermore, large substituent such as phenyl and dimethyl at  $\beta$ -position for  $\gamma$ -((acetyloxy)-methyl)- $\gamma$ -butyrolactone were not accepted as substrate 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 by molecular modeling. The Umbrella like inversion in  $\gamma$ -position can account for the experimental results.



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## **The efficient siRNA delivery system with polymer conjugated lipid nanoparticles assisted by dextran siRNA conjugates**

오미화, 김지선, 박태관

KAIST 생명과학과

Therapeutic siRNA has been exploited as one of the most promising personal medicines in past decades. However, stable delivery of siRNA the most significant issue to overcome is still remained. In that sense, technologies to develop a novel carrier and to engineer siRNA such as PEGylation, lipid conjugation or multimeric siRNA system have been proposed. Here, we suggest a novel siRNA structure, Dextran-siRNA conjugates(DSC), which showed a good serum stability and strong polyplex formation with several cationic carriers including lipid nanoparticles. Lipid nanoparticles( LNP) have been widely studied for effective gene transfection. In particular, natural LDL nanoparticles were employed for plasmid DNA delivery by incorporating with stearyl-poly(L-lysine) as a cationic surface modifier. Besides, LDL mimetic system for siRNA delivery was suggested by our group, which presented excellent gene silencing. These particles with dioleoylphosphatidylethanolamine (DOPE) or 3 $\beta$ -[N-(N', N'-dimethylaminoethane)-carbamoyl]-cholesterol (DC-chol), however, are potentially cytotoxic. Thus, it is essential that DOPE and DC-chol should be substituted with the alternative cationic lipids of low cytotoxicity. Here, we demonstrated new cationic lipid nanoparticles for siRNA carrier that reconstituted from cholesterol conjugated linear PEI of 2.5 KDa and deoxycholic acid conjugated chitosan of 4 KDa. Our LNP is prepared by modified solvent-emulsification method. The size of particle is  $130.65 \pm 0.83$  nm with DLS and the surface charge is evaluated as  $49.47 \pm 6.26$  mV. This DSC/LNP system could provide excellent cellular uptake and gene silencing effects in vitro. It is expected that further modification with various target moieties might induce site specific delivery of siRNA at the next work.

일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: IV-BIO.P-170

발표분야: 생명화학

발표종류: 포스터, 발표일시: 금 15:00~17:00

## Single-molecular FRET study of NSAP1 (hnRNPQ1) and Hepatitis C virus IRES RNA : The dynamics of RNA binding proteins

정현석, \*김병현

포항공과대 시스템생명공학부 \*포항공과대 화학과

Hepatitis C Virus (HCV) Internal ribosomal entry site (IRES), located in the 5' untranslated region directly regulates HCV RNA translation. HCV IRES dependent translation needs noncanonical translation initiation factors called as ITAFs (IRES specific transacting factors). These ITAFs are commonly RNA binding proteins and play important roles in HCV IRES translation. Interestingly, one of ITAF, NSAP1, or heterogeneous nuclear ribonucleoprotein Q1 (hnRNP Q1) augments HCV IRES dependent translation through the specific interactions between hnRNPQ and adenine rich RNA (ACR) in the downstream region of initiation codon (AUG) of HCV IRES. However, the detail mechanisms of ITAFs including NSAP1 for elevating translation efficiency in IRES RNA were not clear until now. Interestingly, NSAP1 binds the downstream site of AUG codon, or the coding region of HCV, not 5' NTR region and it may be expected to recruit other canonical translation factors for the efficient translation. The binding of NSAP1 to ACR is the first important step for enhancing the HCV IRES mediated translation as an ITAF. To investigate NSAP1 binding on HCV IRES ACR and for elucidating NSAP1 binding mechanism on HCV IRES ACR, it is required for direct and subtle monitoring methods for NSAP1. Here, we developed single molecular FRET system and measured direct binding between NSAP1 and HCV IRES ACR. This method can unveil NSAP1 behavior on ACR and allow detailed investigation of RNA binding proteins with specific RRM s on RNA templates. We investigated here the motion of NSAP1 at single molecular level in sequence dependency.

일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: IV-BIO.P-171

발표분야: 생명화학

발표종류: 포스터, 발표일시: 금 15:00~17:00

## Synthesis and Biological Evaluation of Isoxazol-5(4H)-one Derivatives as a New Family of PTP1B Inhibitors with Anti-Obesity Effect

**Kafle Bhooshan, khadka deegendra, Aher Nilkanth G., 조형진**

인하대 화학과

We constructed an isoxazolone chemical library of 70 compounds using a simplified procedure that circumvents tedious work up and purification procedures. The reaction products were obtained as precipitates. The products were purified by a brief washing, which were pure enough for enzymatic experiments. These compounds inhibited PTP1B at submicro molar concentrations. Among them, compound C3 was the most potent inhibitor of PTP1B with an IC<sub>50</sub> of 2.3  $\mu$ M. In vivo effect of C3 was also examined in an obesity-prone mouse strain. The C3-fed mice group gained significantly less weight compared to the control group during the 4 weeks of drug feeding period. In contrast to the anti-obesity effect of C3, no difference was observed in glycemic control between the HFD and HFD + C3 mice groups.

일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: IV-BIO.P-172

발표분야: 생명화학

발표종류: 포스터, 발표일시: 금 15:00~17:00

## Anti-Obesity Effect of a Difuranyl Methylenedisalicylic acid SA37

khadka deegendra, Kafle Bhooshan, Aher Nilkanth G., 조형진

인하대 화학과

Methylenedisalicylic acid (MDSA) derivatives were previously reported as inhibitors of protein tyrosine phosphatase including PTP1B, a therapeutic target for obesity and diabetes. Some of them were also known to inhibit IKK $\beta$ , which is validated target for the treatment of obesity and diabetes. A difuranyl MDSA derivative, SA37, was identified as an inhibitor of both PTP1B and IKK $\beta$  with IC<sub>50</sub> value 67 and 0.62 $\mu$ M, respectively. SA37 was examined for its in vivo effect in mouse model system (C57BL/6J Jms Slc, male). On feeding SA37 to diet induce obese mice significant reduced body weight gain was observed.

일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: IV-BIO.P-173

발표분야: 생명화학

발표종류: 포스터, 발표일시: 금 15:00~17:00

## Detection and Genotyping of Multidrug-Resistant *Mycobacterium tuberculosis* by DHPLC

김진호, \*장원철, 안영창, 조민호, 윤일규, 김정하, 문명진

단국대 화학과 \*단국대 첨단과학대학

In recently years, multidrug-resistant *Mycobacterium tuberculosis* (TB) is a growing concern worldwide. Therefore, there is an increasing important for simply, rapid, specific and sensitive diagnostic methods for detection of MDR-TB. This study illustrates the use of denaturing high performance liquid chromatography (DHPLC) in wild type TB(H37Rv) and other types such as *embB*, *pncA*, *rpsL*. DHPLC is sensitive, specific and possible identify. DHPLC has been applied clinically for mutation(substitution, insertion, deletion) detection and genotyping, that is a relatively technique utilizing heteroduplex formation between wild-type and mutated DNA strands to confirm mutations. As a results, we detected successfully for MDR-TB based on mutations in several specific gene by DHPLC.

일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: **IV-BIO.P-174**

발표분야: 생명화학

발표종류: 포스터, 발표일시: 금 15:00~17:00

## Detection of XRCC1 in Korean Cancer Patients by DHPLC

문명진, \*장원철, 안영창, 조민호, 윤일규, 김진호, 김경하

단국대 화학과 \*단국대 첨단과학대학

The XRCC1(X-ray cross complementing group1) gene is located on chromosome 19q13.2. This gene is interacts with DNA ligase III, polymerase beta, poly (ADP-ribose) polymerase, polynucleotide kinase and AP endonuclease I to participate in the base-excision repair pathway. Arg194Trp, Arg280His and Arg399Gln polymorphisms of XRCC1 has been investigated widely on cancer risk. However Arg194Trp polymorphism do not appear in Asians. In this study, we detected of polymorphisms Arg280His, Arg399Gln from korean cancer patients(Lung Cancer, Breast Cancer and Colorectal Cancer). The DNA extraction from FFPET(Formalin Fixed Paraffin Embedded Tissue) and genotypes were determined by PCR-RFLP assays and Denaturing High Performance Liquid Chromatography(DHPLC). As a results, Arg280His and Arg399Gln polymorphisms is significantly increased the risk of cancer. We detected polymorphisms of Arg280His and Arg399Gln by high specificity and high efficiency DHPLC.

일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: IV-BIO.P-175

발표분야: 생명화학

발표종류: 포스터, 발표일시: 금 15:00~17:00

## Analysis of SUMO4 Gene Polymorphisms in Behcet's Patients by DHPLC

김경하, \*장원철, 안영창, 조민호, 윤일규, 김진호, 문명진

단국대 화학과 \*단국대 첨단과학대학

Small ubiquitin-like modifier 4(*SUMO4*) is a protein that in humans is encoded by the *SUMO4* gene. This protein is located in the cytoplasm and specifically modifies I $\kappa$ B $\alpha$ , leading to negative regulation of NF- $\kappa$ B transcription activity. *SUMO4*, located on chromosome 6p25, have been shown to be associated with several autoimmune diseases. Recently, Behcet's disease(BD) have been shown to be clearly associated with genetic effects as well as with other autoimmune diseases. In this study, we examined the association of *SUMO4* polymorphisms with BD. Genotyping for *SUMO4* haplotype 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, DHPLC is highly sensitive, specific and rapid technique with particularly high potential for the analysis of *SUMO4* haplotype polymorphisms.

일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: IV-BIO.P-176

발표분야: 생명화학

발표종류: 포스터, 발표일시: 금 15:00~17:00

## Isolation of c-reactive protein from human serum using phosphocholine coated magnetic nanoparticles

최은숙, 김은주, 김현철, 정상원

대구경북과학기술원 나노바이오 연구부

C-reactive protein (CRP) is one of the pentraxin proteins and has five calcium-dependent binding sites for phosphocholine. Two-dimensional (2D) molecular imprinting of CRP on magnetic nanoparticles (MNP) could provide the enhanced binding characteristics of the resulting molecularly imprinted nanoparticle. To do this, a phosphocholine-containing monomer (12-(4-vinylbenzyloxycarbonyl)dodecyl phosphocholine, VPC) was synthesized by sequential introduction of 4-vinylbenzyl and phosphorylcholine groups into 12-hydroxyldodecanoic acid. Methacryloxypropyltrimethoxysilane (MPS) coated magnetic nanoparticle was also synthesized (~50 nm) and then VPC was polymerized to MPC coated MNP by addition of AIBN and stirred for 2 hrs at 70°C. The CRP rebinding to VPC coated MNP was analyzed by ELISA and SDS-PAGE. The surface modification was confirmed by IR, XPS and XRF analysis. The CRP rebinding to molecularly imprinted MNP was increased to 7 folds higher than to the non-imprinted MNP. Keywords: c-reactive protein, molecular imprinting, magnetic nanoparticle.



일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: IV-BIO.P-177

발표분야: 생명화학

발표종류: 포스터, 발표일시: 금 15:00~17:00

## **Multiplexed real-time PCR based on fluorescence polarization for quantification of gene expression**

송하은, \*안대로

고려대 생명공학과 \*KIST 생체과학부

Multiplex Real-time PCR is one of the widespread molecular biology techniques for amplification of multiple gene targets in a single PCR experiment. Here, we introduce a novel multiplex real-time PCR method utilizing fluorescence polarization. We quantified two different mRNA from HeLa cells using the method and compared the obtained result with that by a conventional method.

일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: **IV-BIO.P-178**

발표분야: 생명화학

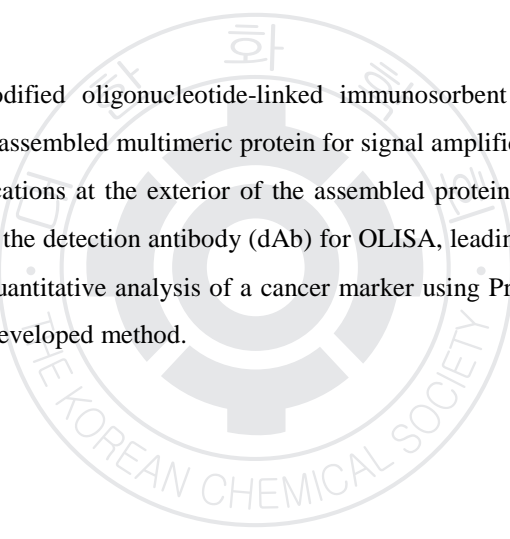
발표종류: 포스터, 발표일시: 금 15:00~17:00

## **Protein assembly for signal amplification in OLISA**

최연경, \*안대로

*KIST 의과학센터 \*KIST 생체과학부*

This study describes a modified oligonucleotide-linked immunosorbent assays (OLISA), so-called Protein-OLISA, using a self-assembled multimeric protein for signal amplification in the immunoanalysis. Chemical or genetic modifications at the exterior of the assembled protein enabled us to conjugate the protein with DNA as well as the detection antibody (dAb) for OLISA, leading to the increased number of DNA sequences per dAb. Quantitative analysis of a cancer marker using Protein-OLISA was performed for evaluation of the newly developed method.



일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: IV-BIO.P-179

발표분야: 생명화학

발표종류: 포스터, 발표일시: 금 15:00~17:00

## **A novel, small molecule inhibitor of HSP70s(Apoptozole) Induce Apoptosis in Cancer cells**

고성균, 신인재

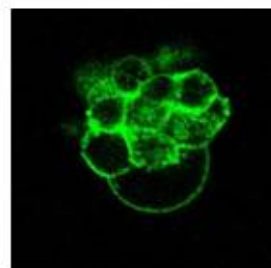
연세대 화학과

Apoptosis (or programmed cell death) is a fundamental biological process that regulates a variety of normal physiological processes, ranging from development to aging. Small molecules that either induce or prevent apoptotic cell death have significant potential as therapeutic agents to treat apoptosis-related diseases. In addition, these agents could also be employed to understand the roles that apoptotic regulatory proteins play in biological processes. Herein we describe a novel apoptosis-inducing small molecule which interacts with Hsc70 and Hsp70. Cell-based screening with a small molecule library is an attractive approach to identify bioactive compounds that regulate protein functions in cells or affect processes such as cell differentiation or morphology. We applied this approach to select molecules with apoptosis-inducing activity, using a recently prepared imidazole library on a solid support to identify bioactive compounds that induce interesting cellular events. The amine-conjugated diethylene glycol linker was introduced into the library for facile solid-phase synthesis and the identification of target protein(s) by affinity chromatography. In conclusion, we have identified from a cell-based assay a small molecule that interacts with Hsc70 and Hsp70. It is likely that this compound induces apoptotic cell death by inhibiting the function of Hsp70 and/or Hsc70, which antagonize apoptosis by interfering with multiple checkpoints in the apoptosis pathways. As an apoptotic inhibitor Az holds considerable potential as a cancer therapeutic and can also be used to further understand the molecular basis of Hsp70-related apoptotic process.

암세포



암세포사멸



*Angew. Chem. Int. Ed.* 2008, 47, 7466



일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: **IV-BIO.P-180**

발표분야: 생명화학

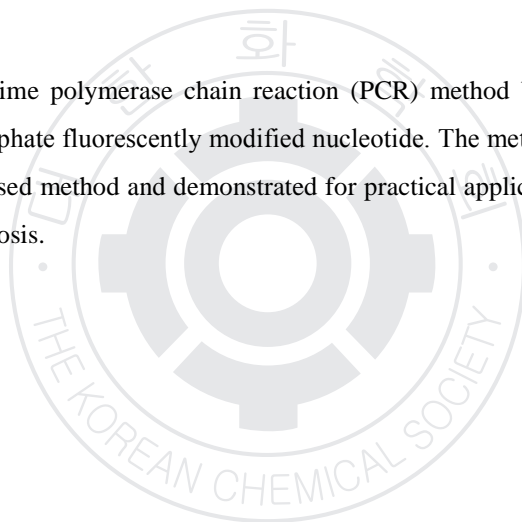
발표종류: 포스터, 발표일시: 금 15:00~17:00

## **A novel real-time PCR method based on signaling-by-incorporation**

송하은, \*안대로

고려대 생명공학과 \*KIST 생체과학부

We describe a novel real-time polymerase chain reaction (PCR) method based on SBI (signaling-by-incorporation) using  $\gamma$ -phosphate fluorescently modified nucleotide. The method has been compared with a SYBR green (SG) dye-based method and demonstrated for practical applications such as quantification of cDNA and malaria diagnosis.



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장소: 제주ICC

발표코드: IV-BIO.P-181

발표분야: 생명화학

발표종류: 포스터, 발표일시: 금 15:00~17:00

## **Heart Malformation is an early response to Small Molecule (Cardiosulfa) in Embryonic Zebrafish.**

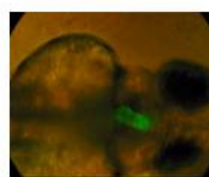
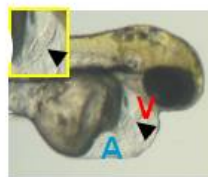
고성균, 신인재

연세대 화학과

Heart disease is one of the most common causes of human death. As a result, a major goal in understanding this disease is the elucidation of mechanisms and pathways that are directly related to the human heart function. The zebrafish has emerged as a powerful model vertebrate for the assessment of heart development owing to the fact that its heart is nearly identical to that of a human embryo at three weeks of gestation. Small molecules that affect developmental processes in zebrafish have been identified by employing the forward chemical genetic approach and used to gain an understanding of the functions of gene products involved in vertebrate developmental events. However, a more intense effort is required to uncover new chemical modulators. As part of a recent investigation aimed at this goal, we have prepared and screened a sulfonamide library designed to identify small molecules that perturb heart development in zebrafish. Herein, we describe the development of a novel, sulfonamide-based small molecule that induces abnormal heart morphology during zebrafish development. We have identified a novel small molecule that impairs zebrafish cardiovascular development and function, and evokes a striking edema response in the pericardial and yolk sac. This compound can be used to unveil mechanism and pathways relevant to heart disease. The observations made in this investigation build upon recent findings that illustrate the value of chemical biology approaches as tools for the elucidation of differentiation and development processes.



제브라피쉬 배아



*Angew. Chem. Int. Ed.* 2009, 48, 7809



일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: **IV-BIO.P-182**

발표분야: 생명화학

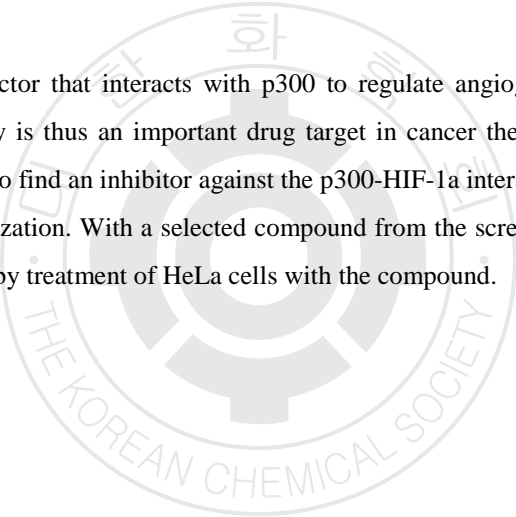
발표종류: 포스터, 발표일시: 금 15:00~17:00

## **An inhibitor for inhibition of the p300-HIF-1a interaction**

권혁성, \*민선준, \*\*안대로

고려대 생명공학과 \*KIST 생체과학연구본부 \*\*KIST 생체과학부

HIF-1a is a transcription factor that interacts with p300 to regulate angiogenesis around cancer cells. Inhibition of HIF-1a activity is thus an important drug target in cancer therapeutics. In this poster, we screened a chemical library to find an inhibitor against the p300-HIF-1a interaction using an in vitro assay based on fluorescence polarization. With a selected compound from the screening, we also examined the potency at the cellular level by treatment of HeLa cells with the compound.





일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: IV-BIO.P-183

발표분야: 생명화학

발표종류: 포스터, 발표일시: 금 15:00~17:00

## Size-dependent Separation of Giant Unilamellar Vesicles Using Pinched Flow Fractionation Devices.

허유희, \*신관우, \*\*이기라

서강대 화학과 \*서강대 화학과 및 바이오융합과정 \*\*충북대 공업화학과

세포막을 구성하는 인지질분자로 이루어진 거대한 Vesicles 인 Giant Unilamellar Vesicle (GUVs)는, 세포의 다양한 생물학적인 특성을 대체하여 연구하기 위한 매우 유용한 구조체이다. 다양한 방법에 의하여 지금이 10 micrometer 이상의 크기로 만들게 되는데, 형성 방법이나 인지질분자의 특성에 따라서 작은 vesicle 이 연구자들이 원하는 크기의 vesicle 까지 섞여서 형성되는 것을 피할 수 없는 문제가 있다. 이를 해결하기 위하여, 기존에 microfluidic chip 의 흐름에 외부의 flow 압력에 의하여 크기에 따라서 분리할 수 있는 device 를 제안한 바 있다. 작은 vesicle 을 분리할 수 있는 channel 을 유속의 수직방향으로 직렬, 혹은 병렬로 연결하여 분리가 가능함을 제시한 바 있다. 그러나, back flow 와 channel 이 막히는 문제를 해결하기 위하여, 최근 새롭게 제안된 원심력에 의한 분리가 포함된 부채꼴 형태의 fluidic device 를 적용하여 GUV 의 분리를 시도하였으며, 기존의 pinched flow 만에 의한 분리와 효과 및 차이점을 소개하고자 한다.

일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: IV-BIO.P-184

발표분야: 생명화학

발표종류: 포스터, 발표일시: 금 15:00~17:00

## Langmuir monolayer of model mitochondrial membrane

Phan Dinh Minh, \*신관우

서강대 화학과 \*서강대 화학과 및 바이오융합과정

Mitochondrion is known as a power-house of human body, where ATP generation is carried out and biological energy is produced. The three major components composing of the mitochondrial inner membrane are phosphatidylcholine (PC, 40% in weight), phosphatidylethanolamine (PE, 40%) and cardiolipin (CL, 20%). The last one, cardiolipin (CL), is a complex phospholipid only found in the energy-transducing membranes of bacteria and mitochondria. It is considered as an essential component in maintaining stability and functionality of mitochondrial membrane. For better understanding, the mixing properties of CL and other phospholipids have been investigated. In this work, we studied the  $\Pi$ -A isotherm of each of mixtures by Langmuir Blodgett method, and calculated out the thermodynamic properties such as excess area, Gibb free energy of mixing and compressibility. In order to clarify how CL amount affect to the 2D-membrane systems, the mixtures which have low content of CL have been picked up for further examining. We used Brewster angle Microscopy (BAM) and Atomic force Microscopy (AFM) to observe domain and phase separation. Furthermore, the structure of molecular layer on liquid and solid subphase has been measured by X-ray reflectivity, especially pointed out the change of structure from low surface pressure – gas phase, to high surface pressure – condensed phase.

일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: IV-BIO.P-185

발표분야: 생명화학

발표종류: 포스터, 발표일시: 금 15:00~17:00

## Mimicking of Cellular Organelle Membrane Structures in an Artificial Cellular Vesicle

이두호, \*이기성, \*\*신종식, \*\*\*신관우

서강대 화학과 \*세화고 \*\*광영고 \*\*\*서강대 화학과 및 바이오융합과정

It is very difficult to define “how a living organism maintains its life”, due to its vast complex disciplines, including its structure, function, growth, origin, and evolution. However, there are many progresses in cell biology, by narrowing the target to an individual cell, which is a building block to compose all living things. Therefore, mimicking structural and functional “artificial cells” can open a new horizon in biophysics, since a cell is also considered to be the basic unit in many pathological processes. Current achievements of researches in mimicking cellular structures are including 1) assembling cellular membranes, composed of mainly phospholipids, and 2) determining the cytoplasmic skeletons, and it will provide a key information to produce, at least, physically (viscoelastically controlled) and chemically (lipid based) controlled cellular vesicles when those structures are combined into a single structure. Another important step to produce “artificial cells” is how we can produce cellular organelles (i.e. mitochondria, ribosomes, Golgi, nucleus, etc) in a plasma cellular vesicle. Not like a cell membrane, mostly having a spherical structure, structures of cellular organelles varies greatly, but uniquely. While a nucleus and many vacuoles have a spherical shape, ERs have an interconnected network structure of tubules and vesicles. A mammalian mitochondrion has a double membrane structure (elongated vesicle-like outer membrane and ruptured and folded inner membrane). In this study, we would like to find a way to produce non-spherical organelle membrane structure. We could produce many interesting structures, such as tadpole, snowman, dumbbell and flower shaped vesicles successfully by varying major membrane components, cholesterol, cardiolipins (for inner mitochondria membranes), and various phospholipids. Furthermore, we would like to show that their unique structure can be maintained in large-sized vesicles (mimicking cellular organelles in a cellular vesicle) by using a microinjector.

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발표분야: 생명화학

발표종류: 포스터, 발표일시: 금 15:00~17:00

## A Chemodosimeter approach to fluorescent sensing and imaging of Cyanide and Zinc

김건희, 신인재, \*홍종인, \*\*윤주영

연세대 화학과 \*서울대 화학부 \*\*이화여대 화학과

The ability to detect metal ions with high specificity under physiological conditions is an important criterion that must be met in the design of fluorescent chemosensors for biological and environmental applications. Among the various chemosensors, fluorescent chemosensors present many advantages, including high sensitivity, low cost, easy detection, and suitability as a diagnostic tool for biological concern. First, the cyanide ion is an extremely hazardous material that damages by absorption through the lungs, gastrointestinal track, and skin and can kill mammals upon binding to a heme unit.. Consequently, there a growing interest in sensing the presence of the toxic cyanide anion by coordination or covalent bonds. Second, the development of a fluorescent probe for zinc ion in the presence of a variety of other metal ions has received great attention. These efforts are stimulated by the fact that zinc ion is involved in a variety of physiological and pathological processes.

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발표종류: 포스터, 발표일시: 금 15:00~17:00

## **Inkjet Printing of bio-ink on Pre-determined Patterns**

박혜연, \*신관우

서강대 화학과 \*서강대 화학과 및 바이오융합과정

The purpose of this study is to demonstrate that bio-inks, containing biologically active particles or cells, can be delivered on pre-determined patterns using a commercial inkjet printer. Since ink-jet printer is capable of seeding controlled volumes of the inks at precise places, any cells can be seeded directly onto any target surfaces, providing the shape-size controlled structure, known as a custom designed tissue scaffold. We modified a commercially available piezo-electric printer, allowing biological macromolecules, including cells and large vesicles fed from 8 different cartridges onto a hydrogel-coated surface. We will present our preliminary results, including density control of seeded cells, cell viability and bio-ink formulation, which have to be determined for further bio-technology unitization of ink-jet based tissue engineering.

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발표종류: 포스터, 발표일시: 금 15:00~17:00

## UV Radiated Linear Single DNA Molecule Analysis on Positively Charged Glass Surface

박현승, 강선아, 조규봉

서강대 화학과

We present a method for UV radiated single  $\lambda$ -DNA molecule analysis, utilizing the T4 Endonuclease V (Pyrimidine Dimer Glycosylase). Cyclobutane pyrimidine dimers (CPDs, including thymine dimers) photochemical reactions will occur the UV expose to DNA double strands. T4 DNA Endonuclease nicks DNA at the specific nicking sites consisted by CPDs. Therefore, we recognize that if DNA has much CPDs, DNA double strands will breaks more frequently.

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## Ratiometric fluorescent sensor by $\text{Zn}^{2+}$ -triggered amide tautomerization

백경화, \*김하나, \*\*윤주영, 신인재

연세대 화학과 \*이화여대 나노과학부 \*\*이화여대 화학과

It is still a significant challenge to develop a  $\text{Zn}^{2+}$ -selective fluorescent sensor with the ability to exclude the interference of some heavy and transition metal ions such as  $\text{Fe}^{2+}$ ,  $\text{Co}^{2+}$ ,  $\text{Ni}^{2+}$ ,  $\text{Cu}^{2+}$ ,  $\text{Cd}^{2+}$ , and  $\text{Hg}^{2+}$ . We report a novel amide-containing receptor for  $\text{Zn}^{2+}$ , combined with a naphthalimide fluorophore, termed ZTRS. The fluorescence, absorption detection, NMR, and IR studies indicated that ZTRS bound  $\text{Zn}^{2+}$  in an imidic acid tautomeric form of the amide/di-2-picolyamine receptor in aqueous solution, while most other HTM ions were bound to the sensor in an amide tautomeric form. Due to this differential binding mode, ZTRS showed excellent selectivity for  $\text{Zn}^{2+}$  over most competitive HTM ions with an enhanced fluorescence (22-fold) as well as a red-shift in emission from 483 to 514 nm. Interestingly, the ZTRS/ $\text{Cd}^{2+}$  complex showed an enhanced (21-fold) blue-shift in emission from 483 to 446 nm. Therefore, ZTRS discriminated in vitro and in vivo  $\text{Zn}^{2+}$  and  $\text{Cd}^{2+}$  with green and blue fluorescence, respectively. Due to the stronger affinity,  $\text{Zn}^{2+}$  could be ratiometrically detected in vitro and in vivo with a large emission wavelength shift from 446 to 514 nm via a  $\text{Cd}^{2+}$  displacement approach. ZTRS was also successfully used to image intracellular  $\text{Zn}^{2+}$  ions in the presence of iron ions. Finally, we applied ZTRS to detect zinc ions during the development of living zebrafish embryos.

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발표종류: 포스터, 발표일시: 금 15:00~17:00

## Antiresorptive and anabolic activity of KIY-0115, a derivative of diptoindonesin G

이선희, \*김익연, \*\*김성환

과학기술연합대학원대 의약 및 약품화학 \*연세대 약학과 \*\*한국화학연구원 화학유전체 연구실

An imbalance between osteoclast-mediated bone resorption and osteoblast-mediated bone formation is the major cause of bone-related disorders such as osteoporosis. In this study, we identified new small molecule with dual activity, antiresorptive and anabolic activity, by using phenotype-based screening methods, RANKL-induced osteoclastogenesis model using RAW264.7 cells and BMP-2-induced osteoblastogenesis using C2C12 cells, respectively. Interestingly, KIY-0115 (a derivative of diptoindonesin G) dose-dependently inhibited the RANKL-induced activity of tartrate-resistant acid phosphatase (TRAP; a biomarker of osteoclastogenesis). Additionally, it significantly enhanced the BMP-2-induced activity of alkaline phosphatase (ALP; a biomarker of osteoblastogenesis) in a dose-dependent manner. These results suggested that the chemical structure of KIY-0115 might be useful to design antiosteoporotic agent with dual activity.



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발표종류: 포스터, 발표일시: 금 15:00~17:00

## Anti-metastatic activity of KY-04004: it inhibits MMP-2 activity and migration of human lung cancer A549 cells

유병준, \*김성호, \*\*이혁, \*\*\*박미경, \*\*\*\*김서현, \*\*\*\*\*김성환

한국화학연구원 약리활성연구센터 \*한국화학연구원 의약화학연구센터 \*\*한국화학연구원 신약연구단 \*\*\*한국화학연구원 약리활성연구부 \*\*\*\*한국화학연구원 신물질연구본부 약리활성연구센터 \*\*\*\*\*한국화학연구원 화학유전체 연구실

In the previous study, anti-cancer activity of KY-04004 has been reported by using xenograft model, but its anti-metastatic potential has not been studied yet. Therefore, we evaluated the effect of KY-04004 on the activity of matrix metalloproteinase (MMP)-2 and migration in human lung cancer A549 cells. In the gelatin zymography analysis and boyden chamber-based cell migration assay, KY-04004 dramatically reduced the activity of MMP-2 and also dose-dependently inhibited the migration of A549 cells. To investigate the mechanism of action, the effect of KY-04004 on the activities of NF- $\kappa$ B and  $\beta$ -catenin was further evaluated by promoter luciferase activity assay. Interestingly, KY-04004 dose-dependently inhibited the activities of NF- $\kappa$ B and  $\beta$ -catenin without any cytotoxicity suggesting that its anti-metastatic activity could result from its potential to regulate the cross-talk between NF- $\kappa$ B and  $\beta$ -catenin signaling pathways. In a further study, its in vivo anti-metastatic activity would be evaluated by using B16F10-inoculated lung metastasis mouse model.

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발표종류: 포스터, 발표일시: 금 15:00~17:00

## Inhibitory effect of KY-03221 on TGF- $\beta$ -induced wound healing via Wnt signaling in human lung cancer A549 cells

박승연, \*신희숙, \*\*박미경, \*\*\*김서현, \*\*\*\*김성환

한국화학연구원 약리활성연구센터 \*한국화학연구원 신물질연구단 \*\*한국화학연구원 약리활성연구부 \*\*\*한국화학연구원 신물질연구본부 약리활성연구센터 \*\*\*\*한국화학연구원 화학유전체연구실

Anti-cancer activity of KY-03221 via the blockade of PI3K/AKT pathway has been recently reported, but its metastatic potential has not been studied yet. Therefore, in this study, we evaluated the effect of KY-03221 on matrix metalloproteinase (MMP)-2 activity via NF- $\kappa$ B and TGF- $\beta$ -induced wound healing via  $\beta$ -catenin signaling that are important phenotypes in cancer metastasis. In the gelatin zymography analysis and NF- $\kappa$ B luciferase reporter assay, KY-03221 did not affect MMP-2 activity and NF- $\kappa$ B activity, but it dose-dependently inhibited TGF- $\beta$ -induced wound healing and  $\beta$ -catenin activity in human lung cancer A549 cells suggesting that KY-03221 might regulate the EMT (epithelial-mesenchymal transition) process in cancer metastasis. In a further study, its precise mechanism of action including cadherin switch would be studied.

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## Identification of small molecule, 6P-47 with anti-resorptive and/or anti-inflammatory activity

이선희, \*김서현, \*\*백승화, \*\*\*배수정, \*\*\*\*민용기, \*\*\*\*\*김성환

과학기술연합대학원대 의약 및 약품화학 \*한국화학연구원 신물질연구본부 약리활성연구센터  
\*\*한국화학연구원 약리활성연구실 \*\*\*한국화학연구원 약리활성연구센터 \*\*\*\*한국화학연구원 생  
명화학연구단 \*\*\*\*\*한국화학연구원 화학유전체 연구실

Osteoporosis and rheumatoid arthritis are the two major obstacles of life for senior citizens. These diseases show different aspects, but the transcription factor NF- $\kappa$ B seems to be their fundamental denominator to control disease-specific events by regulating the expression of genes related with osteoclastogenesis in bone and inflammation in synovial joints. Therefore, we developed NF- $\kappa$ B promoter luciferase activity assay system in RAW264.7 cells and identified small molecules with anti-resorptive or anti-inflammatory activity by treating RANKL or LPS, respectively. Among 877 compounds, 6P-47 compound isolated from Asteraceae, which has been used as an herbal medicine or functional food to treat inflammatory diseases. 51 compounds showed osteoclast inhibition activity, 22 compounds anti-inflammatory activity. Without cytotoxicity, 6P-47 significantly inhibited the RANKL-induced formation of multinucleated osteoclasts and TRAP activity. In the further study, its mechanism of action will be elucidated.

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발표종류: 포스터, 발표일시: 금 15:00~17:00

## **Gold nanoparticle enhanced oligonucleotide-linked immunosorbent assay for sensitive detection of prostate specific antigen**

한기철, \*안대로, \*\*양은경

*KIST 의과학센터 \*KIST 생체과학부 \*\*KIST 의과학연구센터*

Sensitive detection of cancer biomarkers is critical for early detection of cancer. Despite the prevalent use of the conventional enzyme-linked immunosorbent assay (ELISA) in pursuit of detecting cancer biomarkers, simple, sensitive assays are still in demand in the clinical area. Here, we present a gold nanoparticle-mediated oligonucleotide-linked immunosorbent assay (GNP-OLISA) using the microwell plate-based system similarly as in ELISA. Signal amplification in GNP-OLISA is achieved by employing streptavidin-coated nanoparticles for capturing a large amount of biotinylated DNA molecules, followed by iterative cycles of RNA/DNA duplexation and degradation of RNA probe in the duplex by RNase H. The feasibility of GNP-OLISA is demonstrated by performing the assay for prostate specific antigen (PSA), resulting in improvement of the limit of detection by 30 fold over ELISA (supported by the Functional Proteomics Center).

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## Co-delivery of gene and drug using amphiphilic peptide of R3V6 and R3L6

박지환, \*이민형

한양대 생명공학과 \*한양대 응용화학생명공학부

Gene therapy depends on the development of an efficient, non-toxic gene delivery system. In this study, R3V6 or R3L6 peptide, composed of three arginines and six valines or six leucines were synthesized and characterized as DNA and drug co-delivery carriers. These peptides formed self-assembled micelle in aqueous solution with a cationic arginine surface and a hydrophobic valine or leucine core. The peptide micelle had a hydrophobic core, hydrophobic drug may be loaded into the core of the micelle. The incorporation of hydrophobic drug into the core of the peptide micelle has two effects. First, the micelle will be more stable with a tighter core in the presence of hydrophobic drug, which will increase the transfection efficiency. Second, the drug will be delivered into the cells more efficiently by endocytosis of the micelle rather than simple diffusion. In vitro transfection assay with the mixture of hydrophobic drug, BCNU, and the peptide micelle into HEK 293 cells and Neuro2A cells showed that the transfection efficiency of the micelle was improved compared with the micelle without BCNU, suggesting that incorporation of hydrophobic drug increased the stability of the peptide micelle. BCNU and the peptide mixture had the highest transfection at a 0.8:1 weight ratio (BCNU:R3V6) and a 1.2:1 weight ratio (BCNU:R3L6). In conclusion, the R3V6 and R3L6 peptides with BCNU may be useful for anti-cancer drug and gene combinational therapy.

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## Supramolecular fishing for plasma membrane proteins using an ultrastable synthetic host–guest binding pair

이돈욱, \*박경민, 서경원, 정현태, N. Selvapalam, 류성호, 김기문

포항공과대 지능초분자연구단, WCU 첨단재료과학부, 화학과, 분자생명과학부, 시스템생명공학부 \*Harvard university, U.S.A.

Membrane proteomics, the large-scale global analysis of membrane proteins, is often constrained by the efficiency of separating and extracting membrane proteins. Recent approaches involve conjugating membrane proteins with the small molecule biotin and using the receptor streptavidin to extract the labelled proteins. Despite the many advantages of this method, several shortcomings remain, including potential contamination by endogenously biotinylated molecules and interference by streptavidin during analytical stages. Here, we report a supramolecular fishing method for membrane proteins using the synthetic receptor–ligand pair cucurbit[7]uril–1-trimethylammoniomethylferrocene (CB[7]–AFc). CB[7]-conjugated beads selectively capture AFc-labelled proteins from heterogeneous protein mixtures, and AFc-labelling of cells results in the efficient capture of membrane proteins by these beads. The captured proteins can be recovered easily at room temperature by treatment with a strong competitor such as 1,1'-bis(trimethylammoniomethyl)ferrocene. This synthetic but biocompatible host–guest system may be a useful alternative to streptavidin–biotin for membrane proteomics as well as other biological and biotechnological applications.

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## Cellular adhesion behavior on vertical silicon Nanowires

김소연, \*Jellert Gaublonme, \*Hongkun Park, 양은경

*KIST 의과학연구센터 \*Department of Chemistry, Harvard University, USA*

Live cell can response to various environmental factors through direct interactions with adhesion receptors. The focal adhesions reorganize cytoskeleton by complex signal network, which leads to changes in its morphology dynamics, and behavior. Vertical silicon nanowires (SiNWs) penetrating living mammalian cells have previously been found to support cell cultures, as well as to act as a universal platform for probing intracellular molecular events. However, how SiNWs can affect cellular responses has yet to be explored. Employing paxillin, vinculin, and actin as representatives of focal adhesion molecules, the present study addresses the effects of SiNWs on the distribution of adhesion-related molecules in cultured cells atop SiNWs. By examining cell spreading behavior along with real-time imaging of the focal adhesion complex and a matrix degrading protease, it would be concluded that cells can survive on SiNWs by adjusting their morphology, adhesion and behavior through actively organizing these molecules.

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## Effect of 2-oxoglutarate analogues on the HIF-specific hydroxylase activity

김정원, \*양은경

KIST 프로테오믹스개발사업단 \*KIST 의과학연구센터

Hypoxia-inducible factor-1 (HIF-1) is an essential transcription factor that responds to hypoxia in cells. HIF-1 $\alpha$  is regulated by two prominent HIF-specific hydroxylases, proline hydroxylase domain (PHD) and factor-inhibiting HIF-1 (FIH-1). In the normoxic condition, proline residues (Pro402 and Pro564) are hydroxylated by PHD2, thereby recruiting von Hippel-Lindau (VHL). VHL acts as an essential component of an E3 ubiquitin ligase. Lysine residues of the recruited HIF-1 $\alpha$  are then ubiquitinated by VHL, and HIF-1 is degraded via the 26S proteosomal pathway. FIH-1, on the other hand, mediates hydroxylation of the asparagine 803 residue of HIF-1 $\alpha$  which is critical for its interaction with transcription factors CBP/p300. When HIF-1 $\alpha$  is hydroxylated by FIH-1, its binding to CBP/p300 is prohibited, leading to inhibition of VEGF. In the hypoxic condition, hydroxylations of proline and asparagine residues do not occur, resulting in stabilization of HIF-1 $\alpha$ . For hydroxylation reactions, co-factors and co-substrates including Fe<sup>2+</sup>, O<sub>2</sub>, ascorbic acid and 2-oxoglutarate are required. Since 2-oxoglutarate analogues are known inhibitors for PHD2, the present study is designed to evaluate the effect of DMOG (dimethyl oxalyglycine) and N-OG (N-oxalyglycine) on the activity of PHD2 and FIH-1, along with HIF-1 $\alpha$  stabilization. (supported by the Functional Proteomics Center)



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## Detecting enzyme activity in live cells by Silicon Nanowires

나유란, \*김소연, \*\*양은경, \*\*\*Jellert Gaublonne, \*\*\*Hongkun Park

프로테오믹스기술개발사업단 프로테오믹스기술개발사업단 \*KIST 의과학센터 \*\*KIST 의과학  
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Cambridge, MA, 02138

Enzyme activity has been generally detected by various methods including spectrophotometric, calorimetric, chromatographic, and radiometric assays. These in vitro methods employ purified enzymes and substrates in various external conditions, which might not necessarily reflect the real enzymatic activity in live cells. To understand the true nature of enzymatic activity dynamics in live cells, enzymatic activity needs to be probed in live cells without disrupting cells' integrity. Here, we have developed a novel assay using minimally invasive silicon nanowires that are vertically grown or fabricated by etching, and demonstrated that activities of phosphatase and protease are readily analyzed in live cells (supported by the Functional Proteomics Center).

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## Neutron Reflection Study on Membrane Fusion Process Mediated SNAREs-membrane Proteins

김희석, \*신관우

서강대 화학과 \*서강대 화학과 및 바이오융합과정

Cellular membrane fusion is one of the most fundamental processes, occurring in living cell during many biological cellular processes, i.e. fertilization and viral infection. When two cells fuse, their membranes are combined, often, mediated by membrane proteins. Exchange of cytoplasmic contents and forming of a single continuous membrane occur thereafter. One of the most well-known membrane fusion proteins is SNAREs (soluble N- membrane fusion proteinethylmaleimide-sensitive factor attachment protein receptors), but its fusion mechanisms during the fusion process are not fully detailed in molecular level. We studied the lipid vesicle fusion on a supported lipid bilayer using by neutron reflectivity, in order to visualize the structural variations (composition and thickness), before and after the fusion. We will discuss the structural changes in a molecular level, which could not been observed in conventional optical microscopy.

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발표분야: 생명화학

발표종류: 포스터, 발표일시: 금 15:00~17:00

## Purification of GTPBP1 for the structural study on mRNA stability

최성진, 송경미, 전위정, 정의영, 이성환, 조현호, 송시명, 반창일

포항공과대 화학과

Circadian rhythm is a fundamental biological phenomenon in living organisms. Especially, mammals adapt to daily changes from photic information through the retina. Nocturnally synthesis of melatonin hormone in the pineal gland is increased. In the rodent pineal gland, the rhythmic production of melatonin depends on the rhythmic activation of the penultimate enzyme, AANAT (arylalkylamine N-acetyltransferase). Expression of AANAT is regulated during the step of post-transcription and translation. hnRNP Q plays an important role in stability and translation of AANAT mRNA. hnRNP Q is trans-acting factor of 3'UTR and 5'UTR of mRNA. Overexpression of hnRNP Q enhances degradation and translation of AANAT mRNA but knockdown of hnRNP Q sustains AANAT mRNA level. Recently, binding of hnRNP Q with GTPBP1 was reported. GTPBP1 has GDP-bound or GTP-bound form. We think that two forms of GTPBP1 are important to regulate expression of AANAT. In this study, we performed bacterial over-expression, purification and crystallization of intact GTPBP1 and truncated GTPBP1 to understand the structural function of GTPBP1. In further study, we will perform expression of GTPBP1 with hnRNP Q to find binding domain between GTPBP1 and hnRNP Q. Finally, we will determine the structure of GTPBP1 with hnRNPQ and GDP/GTP-bound GTPBP1 to understand the function of GTPBP1.

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발표코드: IV-BIO.P-202

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발표종류: 포스터, 발표일시: 금 15:00~17:00

## Selective delivery of doxorubicin to prostate cancer cells using nanoparticles modified by aptamers

조현호, 송경미, 전위정, 정의영, 이성환, 최성진, 송시명, 반창일

포항공과대 화학과

Delivery vehicles to a target are important in drug delivery systems and many delivery substances have been studied widely. In particular, nanoparticles have been issued as one of the best media for drug delivery. Among these, superparamagnetic iron oxide nanoparticles (SPION) are actively used as magnetic resonance (MR) contrast agents and magnetic field-guided drug delivery vehicles for the treatment of many diseases. Thermally cross-linked SPION (TCL-SPION), used for the purpose of in vivo therapy, has some advantages, such as good dispersibility in a physiological medium, biocompatibility, and an anti-biofouling property that prevents the adsorption of plasma proteins or cells onto their surface. Thus, it is possible to apply TCL-SPION, conjugated with targeting ligands, in many drug delivery systems. In this study, to investigate the in vivo application of the dual-aptamer system, both A10 and DUP-1 aptamers were immobilized on the surface of TCL-SPION. Selective cell uptakes and effective drug delivery action of these probes were verified by Prussian blue staining and trypan blue staining, respectively.

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발표코드: IV-BIO.P-203

발표분야: 생명화학

발표종류: 포스터, 발표일시: 금 15:00~17:00

## SAXS analysis and functional study of *Thermotoga maritima* MutS2

정의영, 송경미, 전위정, 이성환, 최성진, 조현호, 송시명, 반창일

포항공과대 화학과

SAXS (Small Angle X-ray Scattering) technique enables to measure structural features on length scales between 1 nm up to several hundred of nanometers by analyzing the scattering pattern from samples. We have reported the solution structure of *Thermotoga maritima* MutS2 (TmMutS2) using SAXS technique. Dimeric TmMutS2 analysis exhibits the nucleotide- and DNA-dependent conformational transitions, showing the constructed ab initio rigid-body modeling. Superimpositions of TmMutS2 SAXS models to Smr (small-MutS related) and ATPase domains of other proteins show the SAXS-based on structural confirmation for TmMutS2 in solution. Non-specific nicking endonuclease activity of TmMutS2 and its Smr domain is inhibited in the presence of ADPnP and enhanced by the addition of TmMutL (*Thermotoga maritima* MutL). Finally, we show that TmMutS2 suppresses the TmRecA-mediated DNA strand exchange reaction in a TmMutL-dependent manner.

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발표코드: IV-BIO.P-204

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발표종류: 포스터, 발표일시: 금 15:00~17:00

## Study on the development of detection method using selected aptamer for ampicillin

송경미, 전위정, 정의영, 최성진, 이성환, 조현호, 송시명, 반창일

포항공과대 화학과

Ampicillin is a beta-lactam antibiotic that has been used extensively to treat bacterial infections since 1961. It acts as a competitive inhibitor of the enzyme transpeptidase, which is needed by bacteria to make their cell walls. Ampicillin has received FDA approval for its mechanism of action. But its side effects such as upset stomach, diarrhea, nausea, vomiting, anxiety, and colitis are, have been serious problem. So, it is important to use suitable amount. Specially, plants and animals treated ampicillin for food have to check permissible level before sales and distribution. In this sense, aptamer against ampicillin which has potential as bio-probe and detection method using this are being researched. Aptamers are single strand DNA, RNA or peptide which have high affinity with target molecules. We selected the ssDNA aptamer candidates by SELEX using magnetic bead. And fluorescence assay is used for selection of aptamers bound to ampicillin with higher affinity and measurement of their dissociation constants. Furthermore, we try to develop the ampicillin detection method using fluorophore and gold nanoparticle. Based on these results, the selected ssDNA aptamer will be able to develop biosensor for detection of ampicillin which is contained in food product.

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발표코드: IV-BIO.P-205

발표분야: 생명화학

발표종류: 포스터, 발표일시: 금 15:00~17:00

## The expression and purification of human NTH1 protein for functional and structural study

전위정, 송경미, 정의영, 이성환, 최성진, 조현호, 송시명, 반창일

포항공과대 화학과

The primary defense of oxidative damage lesions in DNA is the base-excision repair (BER) pathway. The functional study of BER pathway related proteins is very important, because oxidatively induced DNA lesions have been implicated in the etiology of many diseases and in aging. The BER pathway involves many proteins such as NTH1, OGG1, UNG, APE1, and XRCC1. Among the components of the BER pathway, the human endonuclease III (hNTH1) is a DNA glycosylase which specifically cleaves oxidatively damaged pyrimidines in DNA. In this study, we expressed and purified a recombinant hNTH1 for functional and structural study. The hNTH1 full length gene was amplified from human fibroblast cDNA by polymerase chain reaction (PCR). The amplified hNTH1 gene was cloned into modified pET28a vector containing GST gene and transformed into E. coli BL21(DE3) cell for over expression. The transformed hNTH1 E. coli cell was grown in Luria Bertani(LB) broth at 37 °C until the absorbance at 600 nm was reached to 0.6. Expression of hNTH1 was induced by the addition of isopropyl-thio-b-D-galactopyranoside(IPTG) to a final concentration of 0.2 mM. After 16 h at 18 °C, the cultured cells were harvested by centrifugation. The expressed GST fusion hNTH1 was purified by Ni-NTA affinity, TEV protease digestion, ionic exchange, and size chromatography using FPLC. The purified hNTH1 was concentrated to 10 mg/ml and crystallized by hanging-drop vapor diffusion methods.

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발표코드: IV-BIO.P-206

발표분야: 생명화학

발표종류: 포스터, 발표일시: 금 15:00~17:00

## **A Carrier for Combined Delivery of Dexamethasone and Plasmid DNA in an Animal Model of LPS-Induced Acute Lung Injury**

김현아, 이민형

한양대 응용화학생명공학부

Dexamethasone was conjugated to low molecular weight polyethylenimine (2 kDa, PEI2k). Dexamethasone is a synthetic glucocorticoid with potent anti-inflammatory effects. Dexamethasone conjugated PEI2k (PEI2k-Dexa) was evaluated as a combined delivery carrier of dexamethasone and plasmid DNA (pDNA) in an animal model of lipopolysaccharide (LPS) induced acute lung injury (ALI). PEI2k-Dexa/pDNA transfected lung epithelial cells showed higher transfection efficiency than PEI2k or a simple mixture of PEI2k and dexamethasone. In addition, the PEI2k-Dexa/pDNA complex reduced the levels of pro-inflammatory cytokines in LPS activated macrophage cells. The anti-inflammatory effect of PEI2k-Dexa was higher than those of dexamethasone and a simple mixture of PEI2k and dexamethasone. For in vivo study, the PEI2k-Dexa/pDNA complex was administered by intratracheal injection. PEI2k-Dexa had higher pDNA delivery efficiency than PEI2k in the lung. PEI2k-Dexa/EGFP plasmid complex injected lung showed higher EGFP expression than that of PEI2k in ALI mouse model. In addition, PEI2k-Dexa/pDNA administered group decreased TNF- $\alpha$  and IL-6 in the lung tissue homogenates and bronchoalveolar lavage (BAL) fluid compared with the controls. H&E stains showed that PEI2k-Dexa reduced inflammatory reaction in the lung. Therefore, PEI2k-Dexa may be useful for combination gene and drug therapy for ALI.



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발표종류: 포스터, 발표일시: 금 15:00~17:00

## Construction, Purification of rabies virus nucleoprotein (RVNP) & NMR study

우선희, 원호식

한양대 응용화학과

In the case of peptide vaccines, the research that is used by fusing the part of activating T-helper cell has been continued to increase the immunogenicity. In this study, it used one part of the Rabies virus strain ERA nucleoprotein gene (RVNP) known T-cell epitope. This fragment are 378-435 amino acids of RVNP and are composed of 59 amino acids. it was named as R fragment. We did construction in E.coli expression vector to express R fragment in large quantities. The His-tag was expressed in N-terminal of R fragment to facilitate purification. Using this, the sample for NMR experiments was obtained. 2D NMR (COSY, TOCSY, Relaxation experiments(T1, T2, NOE)) and 3D NMR(HSQC-TOCSY, HSQC-NOESY) experiments were accomplished to make complete NMR signal assignments of R fragment. By measuring CD(circular dichroism) spectroscopy, The overall secondary structure of R fragment was examined. R fragment is a portion of vaccines under development and structural elucidation is necessary. In this study, structural analysis by NMR is in progress.

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발표종류: 포스터, 발표일시: 금 15:00~17:00

## The Development of Prostate Cancer Detection with Aptamer

김소연

동국대 화학과

It is important for prostate cancer, which only occurs in men, to be diagnosed at an early stage like other cancers. Nowadays, the PSA test is used for the detection of prostate cancer. For more effective and early diagnosis, a new method of prostate cancer detection using aptamers was developed. Aptamers can be an ideal material which is single-stranded oligonucleic acid that binds to specific target molecules tightly. Aptamers have many advantages over antibodies. First, aptamers can be generated against toxin as well as molecules that do not elicit immune response. Second, aptamers are simply produced by chemical synthesis and very stable to long-term storage. Finally, aptamers are generated by in vitro process called SELEX (Systematic Evolution of Ligands by Exponential Enrichment). SELEX is an ideal technology for selecting a panel of target-cell specific aptamers. In our laboratory, immobilization step of SELEX is performed on the nanoporous silicon chip in sol-gel. This SELEX-on-a-chip is much faster than that of the existing conventional SELEX. In protein-SELEX-on-a-chip, target proteins are incubated with libraries of single-stranded DNA containing an approximately 10<sup>15</sup> random oligonucleotide sequences. Oligonucleotides bound to the target proteins are collected, while the unbound oligonucleotides are washed away. After repetitive cycles of protein-SELEX-on-a-chip, target protein-specific aptamers can be obtained. This technology can generate aptamers which is bound to target proteins or unknown protein on the surface of cells called biomarker with high affinity and specificity. When the aptamer was selected, an affinity test was done to confirm the binding activity between the aptamer and target PSA. Moreover, a plasma separation chip was developed to simply prepare of the blood sample for prostate cancer diagnosis. The final goal was the development of an integrated chip which included as plasma separation chip and a sol-gel chip with the immobilized aptamer.

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발표종류: 포스터, 발표일시: 금 15:00~17:00

## Expression of obesity control protein B4RB2 and structural studies by NMR

최현주, 원호식

한양대 응용화학과

Apolipoprotein is protein component of lipoprotein serum conjoint fat component. This works for lipid transport agent, and the metabolism of lipoproteins are known to play an important role. So, biochemical and immunological study on the trend that is being made. The risk of coronary heart disease is used as an indicator of LDL cholesterol in the blood serum, because the role of transport at high concentration of LDL may cause arteriosclerosis is predicted. Also the protein component, LDL-cholesterol, is contained only apo B-100. So Clinically measuring change of protein is more accurate than change of serum lipid and lipoprotein components in Circulatory diseases. Through the analysis of the antigenic epitopes of the specific monoclonal antibody of Apolipoprotein B-100, B9, we find pB1 that original antigen amino acid sequence of similar peptides apo B-100. B4 was increased its activation to use vaccine by inserting 378~485 amino acid part of known as activating T helper of Ravies virus nucleoprotein in B4. Finally, we expressed proteins, B4RB2. It is necessary that identify the exact B4RB2's structure to provide Future foundation for clinical use. So in this study, using the circular dichroism(CD), NMR experiments, we can gain the distance between the hydrogen nuclei. In addition through distant geometry(GD) and molecular dynamics we will analysis B4RB2's structure.

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발표종류: 포스터, 발표일시: 금 15:00~17:00

## SELEX for development of mental diseases detection

김소연

동국대 화학과

Developing a diagnostic sensor is one of the key issues in ubiquitous personalized diagnostics. Biosensors which can recognize specific small molecules can be used as a detecting sensor for hormones or metabolites related to disease processes. Recently, aptamers have been used as biomarkers for sensor development. 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. In this study, DNA aptamers that bind to cortisol and dopamine were utilized. Cortisol is a steroid hormone secreted by the adrenal gland involved in stress responses and the immune and nervous system, and abnormal levels of cortisol are implicated in several mental diseases. Dopamine is one of the neurotransmitters that are secreted by neurons. Its level in the brain is related to depression and Parkinson's disease. In order to perform high throughput detection of target molecules in human blood, the development of reagents with high affinity and specificity to hormones is crucial and using aptamers can be an excellent candidate for this development. To select aptamers with high affinities for the target, a process called SELEX is widely used. Through several rounds of the modified SELEX procedure, aptamers specific for cortisol and dopamine were isolated from a random ssDNA library containing 1015 ssDNA molecules. DNA aptamers that target biomarkers of depression can serve as a valuable resource for the detection of mental diseases.

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발표종류: 포스터, 발표일시: 금 15:00~17:00

## **The generation of aptamer that bound to xanthine/hypoxanthine related to NHL diagnosis using SELEX**

김소연

동국대 화학과

Non-Hodgkin lymphomas (NHL) is a group of malignancies that arise from lymphoid tissue. Lactate dehydrogenase has been used as an NHL marker, but its accuracy has been unsatisfactory in diagnosis. Hypoxanthine and its oxidative form, xanthine have been found as a urine marker for NHL diagnosis(Unpublished Data). The hypoxanthine and xanthine showed lower concentration in urine samples of NHL patients than urine samples of normal control group. Here, to detect these metabolite in urine sample, aptamer that specifically bind to hypoxanthine and xanthine were developed. SELEX (Systematic Evolution of Ligands by Exponential Enrichment) is the technology to be used for making aptamers. Aptamers are oligonucleotides or peptide molecules that bind to a specific target molecule using SELEX technology. ssDNA aptamers bound to hypoxanthine and xanthine were selected. In this research, I tried to generate aptamers that specifically bind to hypoxanthine and xanthine in urine sample from NHL patients. To generate aptamer for hypoxanthine and xanthine, after the chemicals(hypoxanthine and xanthine) are immobilized to epoxy bead respectively, I performed conventional SELEX. While the SELEX is ongoing, negative SELEX is also conducted for selecting more specific aptamers for hypoxanthine and xanthine once every three round of SELEX. After developing aptamer which bound to hypoxanthine and xanthine, these aptamer will be used for NHL diagnostic chip.

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발표종류: 포스터, 발표일시: 금 15:00~17:00

## Water pollutant aptamer selection for toxicological monitoring

김소연

동국대 화학과

Polychlorinated biphenyls, 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 or even 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. Generally, chemical target was immobilized on super micro-magnetic beads followed by suppressing a library with 1015 diversity oligonucleotides which has a 40-60 random region flanked by constant primer sequence to binding target. After binding, those with affinity against target is selected, purified and amplified by PCR or RT-PCR to give an enriched pool which is suppressed to the next round. Such successive process is repeated several rounds. When it comes to the last round, aptamers will be identified by cloning and sequence analysis. Then those selected aptamers will be tested individually and sometimes post-SELEX modifications are also needed for selection of better aptamers. Hopefully, using alkylphenol aptamers, with the combination of sol-gel materials, an aptamer-based biosensor will be developed for water pollutants detection, which may be from tap water, with specificity. Moreover, the system will also enable researchers to quickly screen large numbers of biological analytes for a variety of purposes, from disease diagnosis to detection of bioterrorism agents. Finally, this novel aptamer-based water pollutant detection sensor system could be applied to the universal detection of water pollutant with high sensitivity.

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발표종류: 포스터, 발표일시: 금 15:00~17:00

## **Efficient intracellular delivery and multiple-target gene silencing triggered by multipodal interfering RNAs**

이태연, 이동기

성균관대 화학과

Specific gene silencing strategy by using RNA interference (RNAi) is a promising future therapeutics against many diseases including cancer and viral infection. Specially, inhibition of multiple target genes is needed to combat against viral infection or cancer, to suppress the escape mutation and to achieve synergistic antitumor effect. Here we report a chemically synthesized, multiple-target gene silencing RNA structure based upon branched, tripodal and quadruple interfering RNAs (tiRNA and qiRNA). The novel structure interfering RNAs could simultaneously silence up to three or four different mRNA by harboring siRNAs. In addition to the multiple gene silencing, tiRNA or qiRNA complexed with cationic delivery reagent showed enhanced intracellular delivery and gene silencing activities, compared with conventional siRNAs. Therefore, we believe that the novel multipodal interfering RNA structures could become powerful tools for the efficient combinatorial RNAi strategy.

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발표종류: 포스터, 발표일시: 금 15:00~17:00

## **The immune desensitizing effect by siRNA upon following dsDNA stimulus**

유재욱, \*홍선우, \*\*김소연, 이동기

성균관대 화학과 \*동국대 의생명공학과 \*\*동국대 화학과

Specific knock-down of cellular gene expression using short, interfering RNAs (siRNAs) has become a powerful tool for functional genomics studies and a promising future therapeutic approach. However, recent studies have revealed that siRNAs can trigger an innate immune response upon intravenous administration in mice and transfection into purified immune cells by upregulating inflammatory cytokine levels. In present study, we introduce that siRNAs can non-specifically desensitize following dsDNA-mediated innate immune responses. The desensitizing effect triggered by siRNA is involved in the regulation of RIG-I like helicases activity which subsequently modulates immune related transcription factors including nuclear factor- $\kappa$ B (NF- $\kappa$ B) and interferon regulatory factor 3 (IRF3). Since normal innate immune responses against various pathogens should be maintained after siRNA based drug treatment, it is essential removing siRNA-mediated immune desensitizing effect. Our finding of a new side-effect triggered by siRNA contributes the caution of development for siRNA based therapeutics



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## Genome-wide analysis of alternative splicing regulation in dsRNA triggered innate immune response

홍선우, \*이동기, \*\*김소연

동국대 의생명공학과 \*성균관대 화학과 \*\*동국대 화학과

Innate immune system is the first line of defense against pathogens and consists of various cellular signal transduction pathways and complex transcriptional programs. It is well known that accurate transcription response to innate immune stimulating molecule is essential for sustaining survival of an organism. However, complete view of genome-wide transcriptional regulation including alternative splicing under innate immune response still remains elusive. We have been pursuing studies on transcriptional response to viral nucleic acids administration and currently make attempt to characterize genome-wide transcription profiles upon dsRNA treatment. In this study, transcriptome-level response to dsRNA was characterized through the genomics approach such as DNA microarray and next generation sequencing technology. In addition to gene level expression dynamics, analysis of RNA-seq data revealed more than one hundred alternative splicing events. We expect that our genome-wide transcriptome data will elucidate transcription regulation mechanism in dsRNA triggered innate immune response.

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발표종류: 포스터, 발표일시: 금 15:00~17:00

## Effects of concatamer on the Growth and Survival of Cancer cells

이태연, 이동기

성균관대 화학과

These days, we believe that Specific gene-silencing using RNAi is a promising future therapeutics against many diseases. And, The inhibition of cancer growth and progression is one of the major challenges facing modern medicine. Despite significant progress in the development of therapies against cancer, only in a few cases are these therapies effective. Because cancer is a complex disease, agents that target a single oncogenic pathway have low efficacy, in addition to allowing the emergence of drug resistance. So, we suggest modified strategy to inhibit growth and survival of cancer cells. Our RNA concatamer which have specific gene silencing activity have high efficiency to kill the cancer cells. And we believe that concatamer inhibit the growth and survival of cancer cells through the dsRNA-dependent protein kinase PKR activation. From these reason, Our RNA concatamer have effective synergy effect which is gene silencing activity and cell toxicity to cancer cell killing. So, Our RNA concatamer have the potential to be applicable to a wide range of cancers. Thus dsRNA-based anti-cancer strategies could be powerful tools for cancer treatment.

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장소: 제주ICC

발표코드: IV-BIO.P-217

발표분야: 생명화학

발표종류: 포스터, 발표일시: 금 15:00~17:00

## Development of anticancer RNAi therapeutics by targeting KRAS gene

김세라, \*김소연, 이동기

성균관대 화학과 \*동국대 화학과

Since the discovery in 1998 by Fire and Mello, RNA interference (RNAi) has proven to be a useful tool in the fields of biotechnology and promising future therapeutic modality. Small interfering RNAs (siRNAs) are used as the molecular trigger of RNAi to specifically block the expression of the genes causing various diseases including cancer. In this study, we chose KRAS as a target gene to develop anticancer siRNA therapeutics. KRAS is a ki-ras2 Kirsten rat sarcoma viral oncogene homolog which is a group of small GTP-binding proteins, and involved in the regulation of cell division. Therefore, by targeting KRAS through the RNAi, we expect repression of tumor survival, proliferation. Because conventional siRNA (19+2) can have many limitations such as off-targeting effect, we developed long antisense DNA hybrid siRNA which has complementary DNA sequences of KRAS mRNA at end of antisense strand. Using these new types of siRNA, we show the improvement of silencing effect.

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발표분야: 생명화학

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## Developing safe siRNA therapeutics against eye disease.

이창한, \*홍선우, \*\*김소연, 이동기

성균관대 화학과 \*동국대 의생명공학과 \*\*동국대 화학과

Small interfering RNAs (siRNAs) are short, double-stranded RNAs with 19 base pairs (bp) that mediate efficient gene silencing in a sequence specific manner by RNA interference (RNAi) pathway. Recently, siRNAs have been regarded as potent drug against eye disease such as Age-related Macular Degeneration (AMD). AMD is a medical condition which usually affects older adults resulting in a loss of vision in the center of the visual field (the macula) because of damage to the retina. It is a major cause of visual impairment in older adults (>50 years). Until now, anti-angiogenic therapy of AMD has been done for treatment. Many researches for AMD treatment have been focusing on the Vascular Endothelial Growth Factor (VEGF) as a target. For instance, Bevasiranib which is a first-in-class siRNA drug designed to silence the genes that produce vascular endothelial growth factor (VEGF), believed to be largely responsible for the vision loss of wet AMD. Bevasiranib was the first therapy based on the Nobel Prize-winning RNA interference (RNAi) technology to advance to Phase III clinical trials. However, recent studies revealed that angiogenesis suppression by siRNA occurred in sequence- and target-independent manners. According to its results, both non-targeted (against non-mammalian genes) and targeted (against VEGF $\alpha$  and VEGFR1) siRNA suppressed choroidal neovascularization (CNV) via cell surface toll-like receptor 3 (TLR3) activation. So, we developed different form of novel siRNA structure, asymmetric siRNA (asiRNA). It has duplexes shorter than 19 bp that could efficiently trigger gene silencing in human cell lines. Importantly, asiRNAs ameliorated the non-specific effects triggered by siRNAs such as saturation of the RNAi pathway and sense strand-mediated off-target silencing. Here, we selected E-selectin as a target against eye disease to test whether asiRNA can silence mRNA levels and avoid TLR3 activation. E-selectin, also known as CD62E, is a cell adhesion molecule expressed only on endothelial cells activated by cytokines. It plays an important part in inflammation. Endothelial adhesion molecules facilitate the entry of leukocytes into inflamed tissues. This promotes neo-vascularization, a process

central to the progression of rheumatoid arthritis, tumor growth and wound repair. So far, we tested 30 types of siRNA & asiRNA sequences to find the most efficient things and 3 sequences were selected as final candidates. They can silence E-selectin mRNA level very sufficiently and their IC<sub>50</sub> values were also as low as 0.1nM. In Addition, 2'-OMe was introduced into several nucleotides of the sugar in a sense strand of asiRNA to increase thermo-stability and gene silencing efficiency. They showed a better activity than non-modified siRNAs. We believe that this asiRNA form will be potent drug molecules for eye disease.



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발표분야: 생명화학

발표종류: 포스터, 발표일시: 금 15:00~17:00

## DEVELOPMENT OF APTAMERS FOR PANCREATIC CANCER USING CELL- SELEX

chaudhari pooja dua, 이동기

성균관대 화학과

Pancreatic ductal adenocarcinoma is a highly aggressive malignancy with a very low median survival rate. There is an urgent need for development of novel pancreatic cancer biomarkers that can facilitate early diagnosis and also help in development of effective therapeutics. In the present study using Cell-SELEX we have developed 2'F modified RNA aptamers for pancreatic cancer cells. To select aptamers that would be targeted to pancreatic cancer cells markers of ubiquitous presence; we employed a novel strategy whereby we selected aptamers for two pancreatic cancer cell lines in one selection scheme. We used Panc-1 and Capan-1 cells for positive selections and normal human pancreatic ductal cell line (HPEDE) for negative selections. With this approach we obtained eight aptamers that binds to Capan-1 and Panc-1 cells with affinity in low nanomolar range. Quantitative PCR and fluorescent microscope based detection was used to study the binding and specificity of these aptamers. Amongst the 8 selected aptamers, SQ2 aptamer was found to bind both Capan-1 and Panc-1 with high affinity, whereas the binding to HPEDE was almost undetectable. Additionally, SQ2 could also recognize Hpaf-1, a pancreatic adenocarcinoma cell line but did not bind to any non-pancreatic cancer cell line tested so far. We further truncated these aptamers to minimize their size. SQ2 length was reduced from 78 to 25 nucleotides without any loss in the affinity. The truncated aptamer was multimerised to further increase the affinity. SQ2 was conjugated to homopolymers of a nucleoside drug to achieve targeted therapeutics. The aptamer drug conjugate could specifically inhibit cell viability of Capan-1 cells but not toxicity was observed in HPEDE cells, suggesting specific uptake by pancreatic cancer cells. The aptamer SQ2 can be used for many more targeted therapeutic approaches and diagnosis of pancreatic cancer.

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발표분야: 생명화학

발표종류: 포스터, 발표일시: 금 15:00~17:00

## Electrochemical Deposition of Polydopamine Films

강경태, \*남윤기, 최인성

KAIST 화학과 \*KAIST 바이오및뇌공학과

Polydopamine films (PolyDA) have been developed to be a universal surface chemical platform that enables covalent linking of biomolecules on various materials. PolyDA can convert any surface into chemically modifiable surface due to its intrinsic adhesiveness and it has been applied to design biofunctional surfaces. It is desired to develop surface patterning techniques for polydopamine films as the site-selective surface functionalization enables us to design various types of biochips and sensors. In this study, we report a novel method for a facile site-selective surface functionalization by electrochemically polymerizing dopamine molecules. The electrochemical polymerization of dopamine molecules was triggered by applying positive voltage (0.5 V) to the electrode surfaces while suppressing reported voluntary polymerization of dopamines by reducing pH of the solution to 6.0. The deposited polymer films exhibited time-dependant increase of the thickness, and subsequent or *in situ* conjugations of biomolecules to the films were implemented. Spatially localized deposition of polydopamine films was possible on patterned metal electrodes, which made it possible to design surface-funtionalized electrodes for biosensor applications.

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장소: 제주ICC

발표코드: II-ORGN.P-196

발표분야: 유기화학

발표종류: 포스터, 발표일시: 목 15:00~17:00

## Potassium organotrifluoroborate 유도체화 연구

송중호, \*김태정, \*\*블라, \*박순혜, \*\*\*이혜진, \*\*\*\*함정엽

강릉대 화학신소재학과 \*KIST 천연물소재센터 \*\*과학기술연합대학원대 Dept.of Med.Chem. \*\*\*

강릉대 화학신소재 \*\*\*\*KIST 천연물소재연구센터

최근 Suzuki-Miyaura cross coupling reaction 에서 trivalent boron 화합물의 단점을 보완한 potassium organotrifluoroborate 가 coupling partner 로 대체되고 있다. 특히 organotrifluoroborate 류 화합물은 이온결합 형태로 일반적인 salt 와 같아 보관이 용이하고, 안정하여 Suzuki-Miyaura cross coupling reaction 에서 사용이 편리하다는 장점이 있다. 더욱이 organotrifluoroborate 가 다양한 조건에서 안정하다는 사실이 알려지면서 기존의 boron 화합물로는 만들 수 없었던 새로운 organotrifluoroborate 유도체 연구가 증가하고 있다. 이에 본 연구진은 organotrifluoroborate 유도체화 연구의 일환으로 haloaryltrifluoroborate 의 유도체화 연구를 수행하던 중 일반적으로 이용되어 온 Heck reaction 조건하에서 haloaryltrifluoroborate 를 사용하여 alkenylaryltrifluoroborate 화합물이 생성되는 것을 발견하고, 이에 대한 연구 결과를 발표하고자 한다.



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발표분야: 유기화학

발표종류: 포스터, 발표일시: 목 15:00~17:00

## A direct route to triazole organotrifluoroborates via 1,3-dipolar cycloaddition and their cross-coupling reactions

볼라, \*송중호, \*\*김태정, \*\*박순혜, \*\*\*이혜진, \*\*\*\*함정엽

과학기술연합대학원대 Dept.of Med.Chem. \*강릉대 화학신소재학과 \*\*KIST 천연물소재센터 \*\*\*  
강릉대 화학신소재 \*\*\*\*KIST 천연물소재연구센터

Over the past decades organotrifluoroborates have been used in many contexts as valuable synthetic precursors in Suzuki-Miyaura reaction due to their stability, inexpensive routes for the preparation. Also, organotrifluoroborates can be functionalized to build molecular complexity, while leaving the B-C bond intact. On the other hand, “Click Chemistry” has emerged as a fast and efficient approach to synthesis of novel compounds with desired function making use of selected ‘near perfect’ reactions. The 1,2,3-triazole ring is regarded as an important pharmacophore in drug discovery research and shown interesting biological properties. During the study of triazole preparation, we found that a scaffold bearing a -BF<sub>3</sub>K at C-4 position in 1,2,3-triazole ring which would represent an attractive functional group target for various synthetic applications. Herein, we are going to report the preparation of 1,4-disubstituted triazole organotrifluoroborates with different functional group tolerance and their subsequent cross-coupling reactions.

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발표분야: 유기화학

발표종류: 포스터, 발표일시: 목 15:00~17:00

## Polymer-Supported Diazotization Reagent in the Synthesis of Pure Arenediazonium Camphorsulfonate Salts

이선미, 이영민, 지기환

울산대 화학과

We have recently synthesized and characterized new stable arenediazonium camphorsulfonate salts. However, the purification was the problem associated with this methodology. Recovering from this problem we have adapted the same method which we have developed for the preparation of arenediazonium tosylate salts which includes the diazotization of aromatic amines in the presence of p-TsOH by using a sodium-free polymer-supported diazotization agent<sup>1</sup> and successfully synthesized a series of pure and stable arenediazonium camphorsulfonate salts. Diazotization of wide range of aromatic amines was easily carried out by stirring of a mixture of appropriate amine, CSA and the reagent 'Resin-NO<sub>2</sub>' at room temperature in AcOH. Prepared arenediazonium camphorsulfonate salts have easily isolated even in a dry state and show excellent thermal stability. Thus they can be kept safely even for a long time until a subsequent transformation is ready.

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발표분야: 유기화학

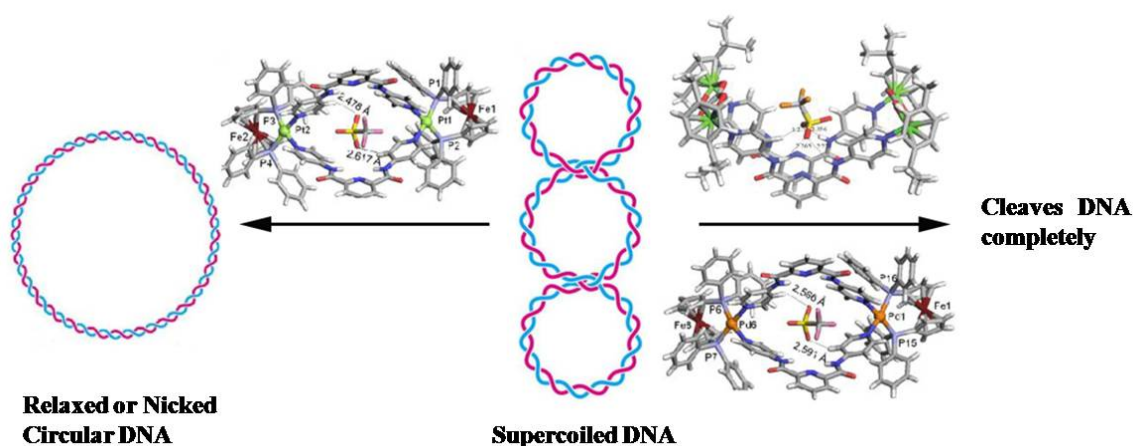
발표종류: 포스터, 발표일시: 목 15:00~17:00

## DNA Cleavage by Supramolecular Metallacycles via Self-Assembly of a bis-Pyridine-amide Ligand and Metal acceptors

ANURAG MISHRA, 정현지, 이혜우, 지기환

울산대 화학과

The present work demonstrates the coordination of the pyridine-amide ligand with different functionality (ferrocene and arene) 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 pyridine-amidic ligands. These self assembled metallacycles were allowed to interact with pUC19 plasmid DNA from *Escherichia coli* for DNA cleavage studies. Agarose gel electrophoresis indicated that the self assembled metallacycles significantly cleave supercoiled (SC) DNA. Results from this work open new avenues for metallacycles in basic and applied bio-science.



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발표분야: 유기화학

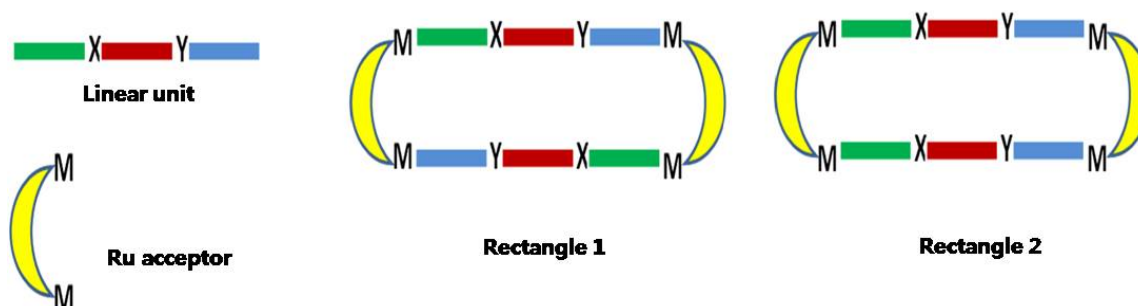
발표종류: 포스터, 발표일시: 목 15:00~17:00

## Self-Assembly of Nanoscopic Rectangles with a New Linear Amide Ligand and Arene Ru-Acceptors

ANURAG MISHRA, 정현지, 송영호, 이해우, 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 chemistry, 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. With the goal of developing a new pyridine-amide ligand that would incorporate two pyridine-N donors and that can allow a large, may be assembled metallacycle by using metal acceptor. Herein, we apply this strategy to the synthesis of a new amide ligand and their coordination chemistry with different arene ruthenium acceptors. These complexes have been characterized by various spectroscopic and X-ray single crystal structure determination. In addition, we used these new rectangles for photoluminescence properties and in future these can be useful in biological applications, particularly for targeting higher-order biological motifs such as selective antitumor therapeutics.



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발표분야: 유기화학

발표종류: 포스터, 발표일시: 목 15:00~17:00

## Self-Assembly of Arene Ruthenium Prismatic Nano-Cages: Synthesis and Photo-physical Studies

vajpayee vaishali, 송영호, 이선미, 지기환

울산대 화학과

Organometallic half-sandwich complexes have been widely used as building blocks in the construction of supramolecular tetra- and hexa-nuclear complexes. We wish to report a set of new ruthenium oxalate bridged prism with tri-pyridyl linker. All the complexes were characterized by  $^1\text{H}$  NMR, ESI-MS and single crystal X-ray analyses of two complexes confirm the formation of these newly synthesized prisms. These prisms showed the selective sensing of nitro-aromatics, in particular TNT and picric acid.

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발표분야: 유기화학

발표종류: 포스터, 발표일시: 목 15:00~17:00

## Self-Assembly of Molecular Rhomboids with Dipyridyl-Carbazole Donor and *cis*-protected Pd and Pt Acceptors

vaipayee vaishali, 송영호, 지기환

울산대 화학과

Two new 2+2 molecular rhomboids were self-assembled by *cis*-protected Pd and Pt acceptors and a newly prepared dipyridyl-carbazole donor. Both the derivatives were well characterized by multi-nuclear NMR and HR-ESI-MS spectral data. The structure of Pd rhomboid was confirmed by x-ray crystallography. These new compounds are highly fluorescent which could be utilized for sensing purpose, so detailed experiments for the sensing of some aromatic guest molecules are in progress.

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발표분야: 유기화학

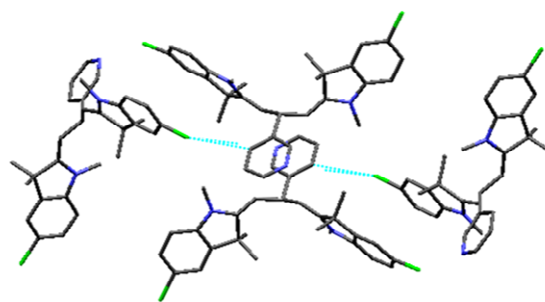
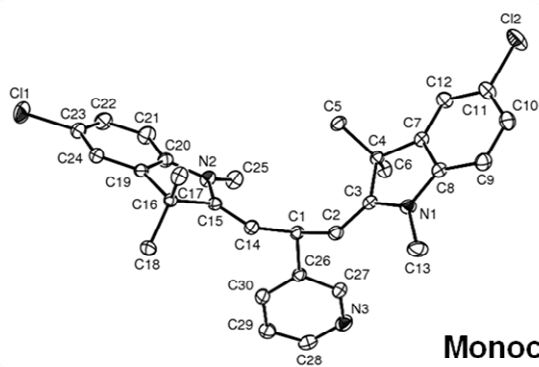
발표종류: 포스터, 발표일시: 목 15:00~17:00

## Stable Structures of Diastereomers of Hetaryl LTAM Molecules Depending on EWD Substituent Group

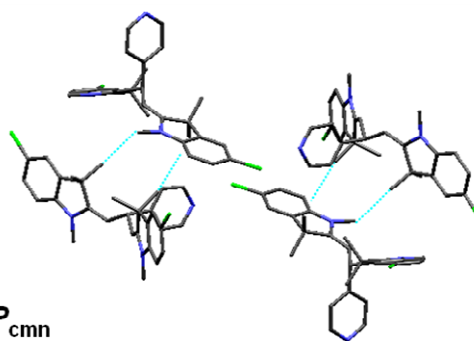
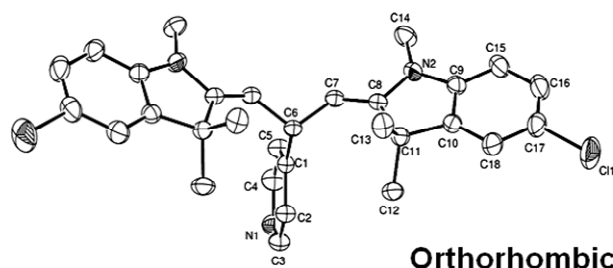
마소영, \*김도경, \*금삼록

고려대 소재화학과 \*고려대 소재화학과

The unequivocal solid-state structure and stereochemistry of the hetaryl leuco-TAM dye, 2,2'-(2-phenyl propane-1,3-diylidene) bis(1,3,3-trimethylindoline) derivatives were established using X-ray single crystal analysis. The X-ray crystal analysis showed that the *ZE*-isomers only formed stereoselectively, with a so-called “three bladed propeller” conformation, from the reaction of a Fischer base and benzaldehyde derivatives. However, the stability and stereoselectivity are completely inverted in the formation of hetaryl LTAM derivatives, when the LTAM molecules contain an electron withdrawing groups such as p-NO<sub>2</sub>, p-(N), p-CHO, etc on the para position of the aryl group. In that situation, the *EE*-isomers unusually are formed mainly and later equilibrated to the mixture of *EE*, *ZE* and *ZZ* isomers. These *EE* isomers were stacked in a juxtaposition to form a dimer of a double dimer, adopting either a triclinic, with P-1, of monoclinic crystal system with a space group P2<sub>1/n</sub> in the unit cell of the crystal.



Monoclinic,  $P2_1/n$



Orthorhombic,  $P_{cmn}$





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발표분야: 유기화학

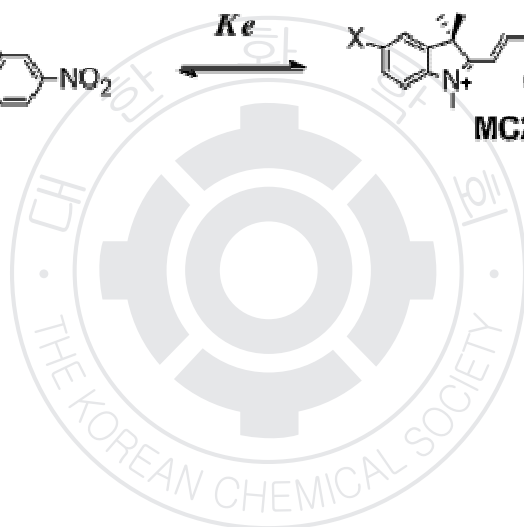
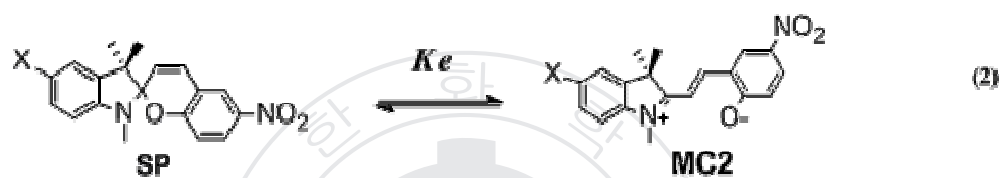
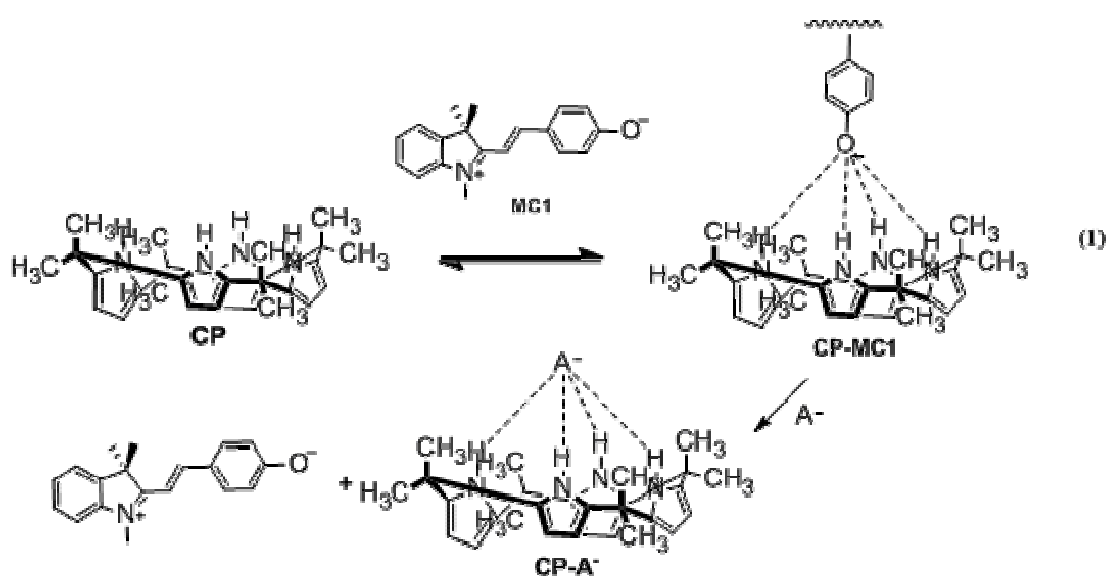
발표종류: 포스터, 발표일시: 목 15:00~17:00

## Complexation between calix[4]pyrrole and the merocyanine form of photochromic spiropyran dyes: determination of the equilibria

임현우, 금삼록

고려대 소재화학과

The interaction between a merocyanine (MC) dye and calix[4]pyrrole (CP) through hydrogen bonding is well known(eq.1). This MC-CP complex can then be destroyed by the anion, such as halogen anion, reforming a Cl<sup>-</sup>-CP complex and a colored MC species. This was verified that the formation of the complex MC1-CP and displacement of the complex with Cl<sup>-</sup> anion with the production of the colored MC species back. It's also very well known that thermo- and photochromic spiropyran is equilibrated with the open-form merocyanine MC2 (eq.2), after exposure to the light. However, equilibrium constants can be hardly obtained since the exact extinction coefficient of MC2 is not known. Thus a new method is applied to get an exact extinction coefficient value of the MC2 species and hence determined equilibrium constant  $K_e$ , utilizing the MC-CP complexation.



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발표코드: II-ORGN.P-205

발표분야: 유기화학

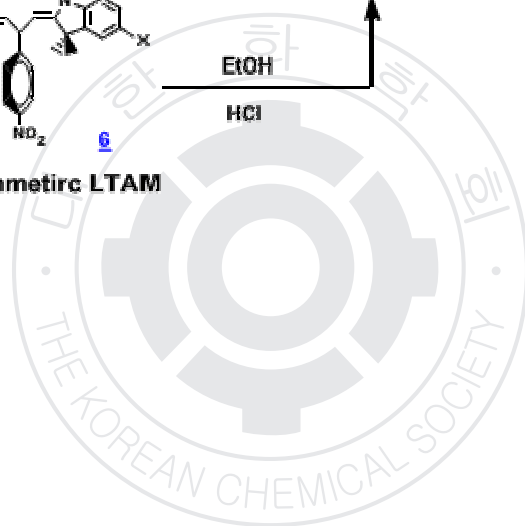
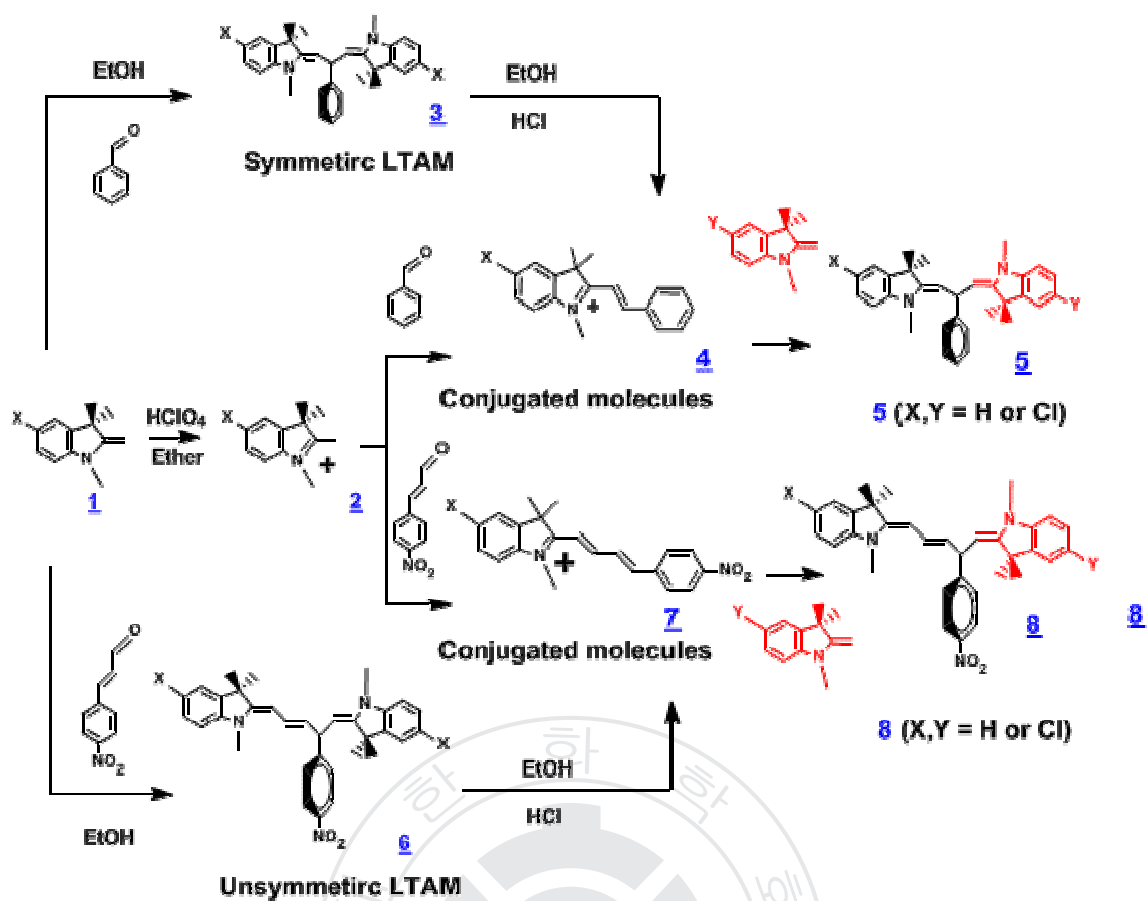
발표종류: 포스터, 발표일시: 목 15:00~17:00

## Synthesis and spectroscopic characterization of unsymmetric leuco-TAM derivatives

김현수, 금삼록

고려대 소재화학과

Novel unsymmetric hetaryl LTAM molecules, (2Z, 2E)-2,2-(2-phenyl-propane-1,3-diylidene)bis(1,3,3-trimethylindoline) 5 and unsymmetric LTAM molecules, (2Z,2'E)-2-2'((E)-4-(4-nitrophenyl)pent-2-ene-1,5-diylidene)bis(1,3,3-trimethylindoline) 8 were prepared from the reaction of excess 5-substituted Fischer base (FB) with the conjugated dye molecules 4 and 7, respectively, via a Michael type reaction. Since the conjugated dye molecules is the  $\alpha$ ,  $\beta$ -unsaturated iminium salts, they behave like an  $\alpha$ ,  $\beta$ -unsaturated carbonyl compounds toward the Michael reaction. The compound 4 & 7 were obtained from the reaction of 1,3,3-trimethyl-2-styrylindolium perchlorate 2 and benzaldehyde or cinnamic aldehyde, respectively. Another route for the conjugated compounds are the acid-catalyzed decomposition of the symmetric LTAM molecules 3 or 6, which was prepared from the Fisher base and the corresponding aldehydes. The prepared molecules were characterized by  $^1\text{H}$ ,  $^{13}\text{C}$ -NMR, IR, UV-Vis spectroscopy.



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장소: 제주ICC

발표코드: II-ORGN.P-206

발표분야: 유기화학

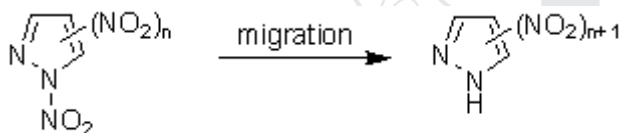
발표종류: 포스터, 발표일시: 목 15:00~17:00

## Studies on the sigmatropic nitro migration of N-nitropyrazoles

이미진, 최준호, 김태근, 정규현

인하대 화학과

The direct nitration of pyrazole, using nitric acid or mixture of nitric acid and sulfuric acid, leads to substitution in the 4 position. 1-Nitropyrazole undergoes intramolecular rearrangement at 120~190°C to form 3(5)-nitropyrazole in high yield. The 1,2-sigmatropic shift of the nitro group is considered as the first step of this rearrangement, which is followed by fast rearomatization of intermediates. Thermal N to C migration of NO<sub>2</sub> is not restricted to pyrazole. Analogous migration were found in N-nitroindazole, triazole, and imidazole. We will discuss thermal rearrangement of N-nitropyrazoles.



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발표코드: II-ORGN.P-207

발표분야: 유기화학

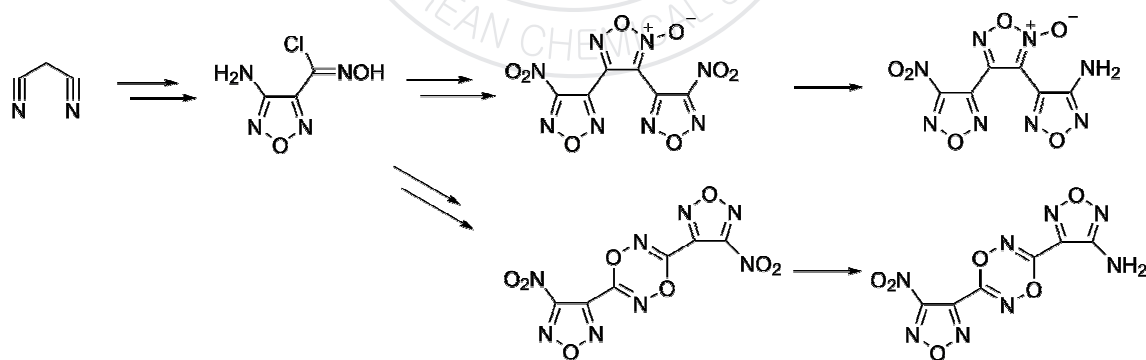
발표종류: 포스터, 발표일시: 목 15:00~17:00

## Studies on the Synthesis and Selective Reduction of Furoxan Derivatives

이병우, 김태근, 정규현

인하대 화학과

The furoxan ring is well known as highly energetic heterocycles. And one of its derivatives, 3,4-bis(nitrofurazano)furoxan (BNFF) has excellent explosive properties such as high thermal stability, density, and higher detonation velocity and pressure comparable to HMX. BNFF and its structural isomer, 3,6-bis(4-nitro-1,2,5-oxadiazole-3-yl)-1,4,2,5-dioxadiazine (BNFOZ) are synthesized from commercially available malononitrile through multiple step. And furthermore we will discuss about selective reduction of BNFF and BNFOZ.



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발표분야: 유기화학

발표종류: 포스터, 발표일시: 목 15:00~17:00

## Synthesis and recognition properties of new rhodamine chemosensors.

최진욱, 장승현

대구대 화학과

New bis-rhodamine 6G was synthesized from rhodamine 6G. New bis-rhodamine was synthesized two steps from rhodamine 6G. Two kinds of new rhodamine were synthesized from rhodamine 6G. The first one is bis-rhodamine and the other one is rhodamine containing. New bis-rhodamine was synthesized from rhodamine 6G and 2,6-pyridinedicarbaldehyde. New rhodamine was synthesized from rhodamine 6G and 2-hydroxy-1-naphthaldehyde. We will present some recent recognition results of fluorescent properties of new rhodamine chemosensors.

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장소: 제주ICC

발표코드: II-ORGN.P-209

발표분야: 유기화학

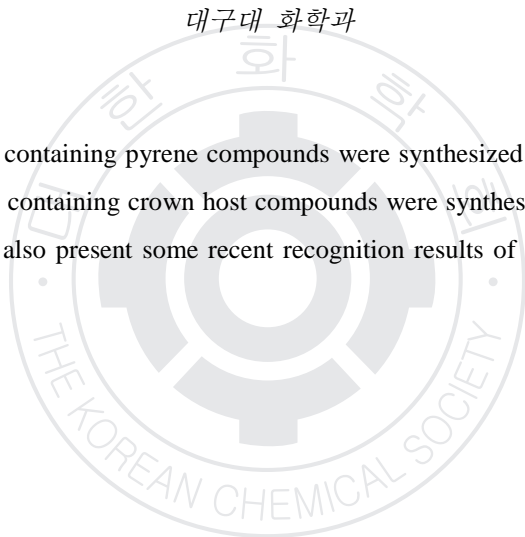
발표종류: 포스터, 발표일시: 목 15:00~17:00

## **Synthesis and recognition properties of new bis-crown ethers containing pyrene moieties.**

주재운, 장승현

대구대 화학과

New kinds of crown ethers containing pyrene compounds were synthesized by pyrene and crown ethers functionalized. Fluorophore containing crown host compounds were synthesized from reaction of pyrene and crown ethers. We will also present some recent recognition results of fluorescent properties of the crown ethers.





일시: 2011년 4월 28~29일(목~금) 2일간

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발표코드: II-ORGN.P-210

발표분야: 유기화학

발표종류: 포스터, 발표일시: 목 15:00~17:00

## Pd-Catalyzed *Ortho*-Methylation of Acetanilides via C-H Activation

장민정, 윤소원

한양대 화학과

Pd-catalyzed C-H activation of arenes has attracted the most attention as an efficient synthetic method due to its atom economy and eco-friendliness. Recently, we reported a highly effective Pd-catalyzed *N*-Ac-directed C-H activation of acetanilides and subsequent C-C bond formation to give a variety of *ortho*-alkenyl acetanilides. In continuation of our interest in Pd-catalyzed C-H bond functionalization, we investigated Pd-catalyzed *ortho*-methylation of acetanilides with methyl iodide. Here, we will present the recent findings.

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장소: 제주ICC

발표코드: II-ORGN.P-211

발표분야: 유기화학

발표종류: 포스터, 발표일시: 목 15:00~17:00

## Facile and Efficient Synthesis of 5,6-Dihydrophenanthridines via Pd-Catalyzed C-H Functionalization

김병석, 윤소원

한양대 화학과

Recently, direct C-H activation of aromatic compounds has attracted the most attention among a variety of synthetic transformations. In this context, we have developed a mild and efficient Pd-catalyzed oxidative coupling reaction between *N*-Ts-2-arylanilines and electron deficient olefins to afford 5,6-dihydrophenanthridine derivatives. In this reaction Pd-catalyzed directed olefination precedes an intramolecular nucleophilic cyclization reaction, leading to a facile and efficient one-pot synthetic route to N-heterocyclic compounds.

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장소: 제주ICC

발표코드: II-ORGN.P-212

발표분야: 유기화학

발표종류: 포스터, 발표일시: 목 15:00~17:00

## **Au(I)-Catalyzed Intramolecular Cyclization Reactions: An Efficient Synthesis of Indenes and Naphthalenes**

장민정, 주진혁, 윤소원

한양대 화학과

In recent years, transition metal catalysis has attracted considerable attention since the reactivities of metal catalyst and/or functional group can be controlled, leading to the construction of various C-C and C-heteroatom bonds. Herein, we present Au(I)-catalyzed intramolecular cyclization reactions of 2-alkenylphenyl carbonyl compounds to give indene or naphthalene derivatives depending on the substitution pattern of alkene moiety.

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장소: 제주ICC

발표코드: II-ORGN.P-213

발표분야: 유기화학

발표종류: 포스터, 발표일시: 목 15:00~17:00

## Calix[4]pyrroles Bearing Two Crossing Straps and Their Anion Binding Chemistry

이창희, 유수연

강원대 화학과

Calixpyrroles and related macrocycles are non-planer synthetic anion receptors that have attracted considerable attentions in recent years. Various modifications have been attempted in order to improve the recognition properties including sensitivity and selectivity. As part of our continuing efforts for these direction, we have now reported new strapped-calix[4]pyrrole systems bearing two crossing straps on either side of the calix[4]pyrrole macrocycle. The synthesis was accomplished by acid-catalyzed condensation of bis-dipyrromethanes and acetone. The condensation afforded three different products. Interestingly, the reaction did not give one of the expected condensation product, namely two diametrical crossing straps. The identity of the products was fully characterized by spectroscopic means including proton NMR, HRMS and single crystal X-ray crystallography. The preliminary binding studies indicate that the receptor bearing two cis-crossing straps are excellent fluoride inclusion receptor with anion/receptor stoichiometry of 1/2. However, the receptor bearing two trans-crossing straps showed fast equilibrium with fluoride anion.

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장소: 제주ICC

발표코드: II-ORGN.P-214

발표분야: 유기화학

발표종류: 포스터, 발표일시: 목 15:00~17:00

## Synthesis and Chemical Properties of non-Aromatic, meso-Alkylidene Schiff-base Macrocycles

이창희, 유화영, 박은화

강원대 화학과

The meso-alkylidenyl porphyrins and related macrocycles are rather recently developed porphyrinoids and have demonstrated unique properties in terms of their tautomerization characteristics and structural features. We present that the synthesis and characterization of meso-alkylidenyl expanded porphyrinoid macrocycles including their Schiff-base analogs. The synthesis of these substances, which all contain unique exocyclic C-C double bonds at multiple meso-positions, have been accomplished by utilizing a typical '3+1' type mixed-condensation. Synthesized compounds displayed unique protonation behavior upon treatment with acids. The initial protonation occurred at the alpha-position of the meso-substituent in most cases. The Schiff-base macrocycles are somewhat resistant to the DDQ-oxidation and resulted in the formation of macrocyclic imines bearing sp<sup>3</sup>-hybridized meso-carbons. The synthesis and physico-chemical properties of the macrocycles as well as protonation selectivity will be presented.

일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: II-ORGN.P-215

발표분야: 유기화학

발표종류: 포스터, 발표일시: 목 15:00~17:00

## **Synthesis and Chemical Properties of meso-Malononitrilidene-(1,3-pyreno)thiaporphyrins and meso-Malononitrilidene-(p-benzi)thiaporphyrins their expanded analogs**

이창희, 유재덕

강원대 화학과

The synthesis and characterization of non-aromatic meso-malononitrilidene porphyrinoid macrocycles and their expanded analogs will be described. The synthesis was accomplished in a straight forward manner by utilizing a typical '3+1' type mixed-condensation. Synthesized compounds contain unique exocyclic carbon-carbon double bonds at multiple meso-positions and showed unique protonation selectivity upon treatment with trifluoroacetic acid. The initial protonation usually occurred at the alpha-position of the meso substituent when diethylmalonylidene group was substituted at meso-position. However, when the meso-substituent is malononitrilidene group, core-protonation and meso-alpha-protonation was competing and formed complex mixture of the protonated species. The meso-malononitrilidene-(1,3-pyreno)thiaporphyrin and meso-malononitrilidene-(1,4-naphthyl)thiaporphyrin was fluorescencet in spite of their non-aromatic character. The newly synthesized porphyrins displayed red-shifted absorption maxima.

일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: II-ORGN.P-216

발표분야: 유기화학

발표종류: 포스터, 발표일시: 목 15:00~17:00

## Aromatic/Antiaromatic Expanded Porphyrinoids Displaying Unique Physicochemical Property

이창희, 김수진

강원대 화학과

New pi-extended, expanded porphyrinoid macrocycles such as naphthorosarin, naphthorubyrin, naphthosapphyrin and naphtha-octaphyrin were synthesized and fully characterized by spectroscopic means including single crystal X-ray diffraction analysis. The 24-pi naphthorosarin exhibited antiaromatic character in spite of its perfect planar structure and global conjugation of double bonds. The most prominent feature in proton NMR spectrum is that the chemical shifts of the core N-Hs appeared at 26.2 ppm, which is unambiguous indication of anti-aromatic character. On the other hand, the two-electron reduced naphthorasarin exhibited typical 26-pi aromatic characteristics. 24 pi-Naphthorosarin became exceptionally stable paramagnetic upon multiple protonation. Naphthorubyrin and naphthosapphyrin, on the other hand, displayed typical aromatic characteristics. These compounds were more basic than other expanded porphyrins. Larger hypsochromic shift of Q-bands upon protonation was observed.

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발표분야: 유기화학

발표종류: 포스터, 발표일시: 목 15:00~17:00

## **(Bezocrown-8)-capped Calix[4]pyrroles: Ion-Pair Receptors Displaying Unique Ion Recognition Properties**

이창희, \*Suman Adhikari

강원대 화학과 \**kangwon National University*

Ditopic ion pair receptors, bearing bezocrown moiety as cation binding site and calix[4]pyrrole as anion-binding sites, have been synthesized and fully characterized. Binding studies confirmed that the synthesized receptors form stable complex with various anions in organic media. The cation binding site, on the other hand, showed selectivity for cesium ion. When the fluoride-bound host was treated with alkaline metal ions, distinctive ion-pair formation with cesium ion was observed. When the fluoride-bound host was treated with Li<sup>+</sup> or Na<sup>+</sup> ion, decomplexation of the bound fluoride was observed. On the contrary, the fluoride complex of simple oligoether-strapped calix[4]pyrrole was treated with Cs<sup>+</sup>, the cation bound to the cup of the calix[4]pyrrole to form receptor-shared ion-pair complex. The chloride-bound host displayed different complexation behavior. Namely, the Li<sup>+</sup> ion bound to the crown moiety to form the contact ion-pair complex. The supramolecular binding properties of the anion-bound hosts will be presented in detail.



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장소: 제주ICC

발표코드: II-ORGN.P-218

발표분야: 유기화학

발표종류: 포스터, 발표일시: 목 15:00~17:00

## Calix[4]pyrrole-Based Fluorescence Indicator Displacement Assay (FIDA) Sensors for Anions and Their Selectivity Tuning

이창희, \*Punidha Sokkalingam

강원대 화학과 \*kangwon national university

A simple and convenient method to quantitatively determine the fluoride anion concentration in organic media has been reported. We designed and synthesized four cis-5,15-(p-X (X= F (1), Br (2), I (3) and CN (4))phenyl)-(5,10,10,15,20,20-hexamethyl)calix[4]pyrrole receptors that bind strongly with fluorescent indicator. The receptor-bound indicator can be replaced when competitive analytes having greater affinity with receptor have been introduced. We found that the highly fluorescent coumarin derivatives strongly bind with synthesized receptors ( $K_a = 4.69 \times 10^6$  (1);  $1.15 \times 10^6$  (2);  $7.11 \times 10^5$  (3) and  $1.16 \times 10^6$  (4)) with complete loss of fluorescence. When these non-fluorescent, host-chromenolate complex were exposed to the mixture of anions, the bound chromenolate anion was displaced more selectively by fluoride anion ( $K_a = 5.96 \times 10^6$ ) with full restoration of fluorescence. While fluoro-substituted receptor showed a greater affinity towards only fluoride anions, the iodo-substituted one exhibited relatively high selectivity for both acetate and fluoride anions. The increase in the fluorescence intensity was found to be closely related with the concentration of added anions. Thus the present work can provide structural foundation for selectively sensing various anions by introducing suitable substituent in the receptor.

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장소: 제주ICC

발표코드: II-ORGN.P-219

발표분야: 유기화학

발표종류: 포스터, 발표일시: 목 15:00~17:00

## 1,3-Dipolar Cycloaddition Reactions of meso-Alkylidene Porphyrins

이창희, 박도우

강원대 화학과

1,3-Dipolar cycloaddition reaction is increasingly popular in the field of the chemical modification of porphyrin skeleton. We applied this reaction to the chemical transformation of meso-alkylidene porphyrins that we have synthesized recently. The reaction of in situ generated azomethine ylide (generated from the reaction of N-methyl glycine with formaldehyde) with diethyl malonylidene-(m-benzi)thiaporphyrin or its expanded analogs afforded cyclized adducts. The reaction took place regioselectively on the pyrrole adjacent to the meso-alkylidenyl double bond. Other regioisomers were also formed as minor products. All the products were identified by spectroscopic means and MOLDI-TOF mass spectrometry. The regioselectivity can be interpreted by the fact that the dipolarophile (porphyrin) must be electron deficient (lower LUMO) for fast reaction. The reaction can be applied to the construction of reduced porphyrins which are useful in various porphyrin-related applications.

일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: II-ORGN.P-220

발표분야: 유기화학

발표종류: 포스터, 발표일시: 목 15:00~17:00

## Anion Binding of Pyrrole-Strapped Calix[4]pyrroles

이창희, 박건유

강원대 화학과

Recently, calix[4]pyrroles and their modified analogs have been actively studied as novel neutral anion-binding receptor since the property was discovered in 1996. Various modifications have been attempted in conjunction with improving the binding affinity as well as selectivity. We have synthesized few pyrrole-strapped calix[4]pyrroles that bear signaling part 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 titled receptor could be excellent fluorogenic anion receptors for anions. The anion selectivity and binding affinity of the receptors will be presented in detail. Also presented will be the functionalization of the synthesized receptor in order to introduce signaling units.

일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: II-ORGN.P-221

발표분야: 유기화학

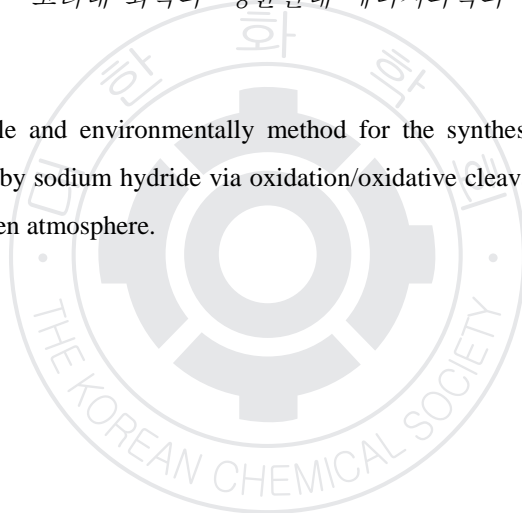
발표종류: 포스터, 발표일시: 목 15:00~17:00

## **Oxidation of benzoin to benzoic acids using sodium hydride under oxygen atmosphere**

강선혜, 한호규, \*양정운

고려대 화학과 \*성균관대 에너지과학과

An efficient, easy to handle and environmentally method for the synthesis of carboxylic acids from benzoin can be proceeded by sodium hydride via oxidation/oxidative cleavage in one-pot procedure has been developed under oxygen atmosphere.



일시: 2011년 4월 28~29일(목~금) 2일간

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발표코드: II-ORGN.P-222

발표분야: 유기화학

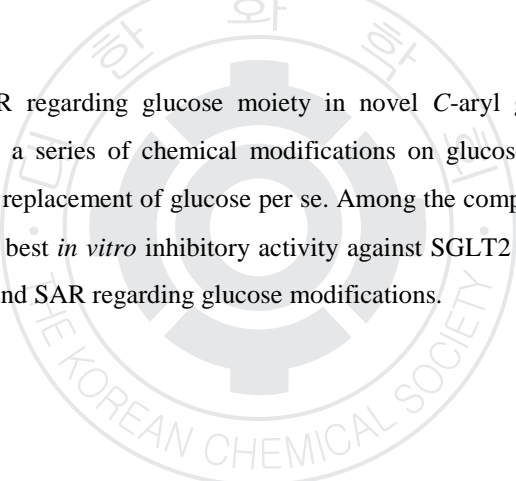
발표종류: 포스터, 발표일시: 목 15:00~17:00

## Exploration of SAR Regarding Glucose Moiety in Novel C-Aryl Glucoside Inhibitors of SGLT2

박은정, 이진화

(주)녹십자 종합연구소

In order to investigate SAR regarding glucose moiety in novel C-aryl glucoside SGLT2 inhibitors containing a thiazole motif, a series of chemical modifications on glucose was conducted to explore potential utility as a suitable replacement of glucose per se. Among the compounds prepared, deshydroxy compound demonstrated the best *in vitro* inhibitory activity against SGLT2 in this series to date. Herein we wish to report synthesis and SAR regarding glucose modifications.



일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: II-ORGN.P-223

발표분야: 유기화학

발표종류: 포스터, 발표일시: 목 15:00~17:00

## **Thiazolylmethyl ortho-Substituted Phenyl Glucoside Library as Novel C-Aryl Glucoside SGLT2 Inhibitors for the treatment of type 2 diabetes mellitus**

이석호, \*김정민, \*이진화

(주)녹십자 종합연구소 의약화학팀 \*(주)녹십자 종합연구소

In order to investigate SAR regarding proximal phenyl ring in novel C-aryl glucoside SGLT2 inhibitors containing a thiazole motif, a series of chemical modifications on proximal phenyl ring was conducted. During a series of lead optimization efforts, some compounds demonstrated subnanomolar inhibitory activity against hSGLT2. The information obtained from the SAR studies in this study might help to design more active SGLT2 inhibitors that are structurally related.

일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: II-ORGN.P-224

발표분야: 유기화학

발표종류: 포스터, 발표일시: 목 15:00~17:00

## Synthesis and Molecular Recognition Properties of Azacalix[4]pyrroles

이창희, 박경화

강원대 화학과

Calix[4]pyrroles are well-known neutral receptors for anionic species and various modifications have been reported recently for enhanced binding affinity and guest selectivity. As part of our efforts for searching a water soluble version of calix[4]pyrrole analogs, we have synthesized new calix[4]pyrroles that bear nitrogen at meso-positions. The identity of the new receptors was characterized by spectroscopic means including proton NMR, HRMS and single crystal X-ray crystallography. The solution-phase binding studies revealed that the receptor could be excellent anion receptors. The anion selectivity and binding affinity of the receptors were studied in detail. Also presented will be the functionalization of the synthesized receptor in order to introduce signaling units.

일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: II-ORGN.P-225

발표분야: 유기화학

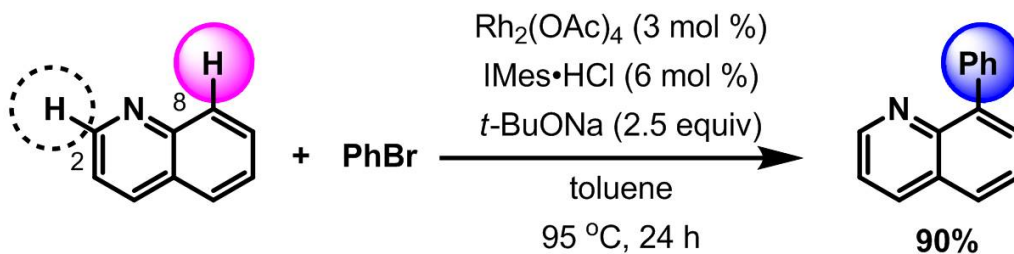
발표종류: 포스터, 발표일시: 목 15:00~17:00

## Rh(NHC)-Catalyzed Direct and Selective Arylation of Quinolines at the 8-Position

곽재성, \*김민, 장석복

KAIST 화학과 \*University of California, San Diego, USA

A new catalytic protocol for the regioselective direct arylation of quinoline derivatives at the 8-position has been developed. The reaction is catalyzed by a Rh(NHC) system, and the choice of the NHC ligand was most important for achieving high reactivity and selectivity.



- **Highly Regioselective**
- **Mild Reaction Conditions**
- **No Pre-Activation**
- **No Directing Group**



일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: II-ORGN.P-226

발표분야: 유기화학

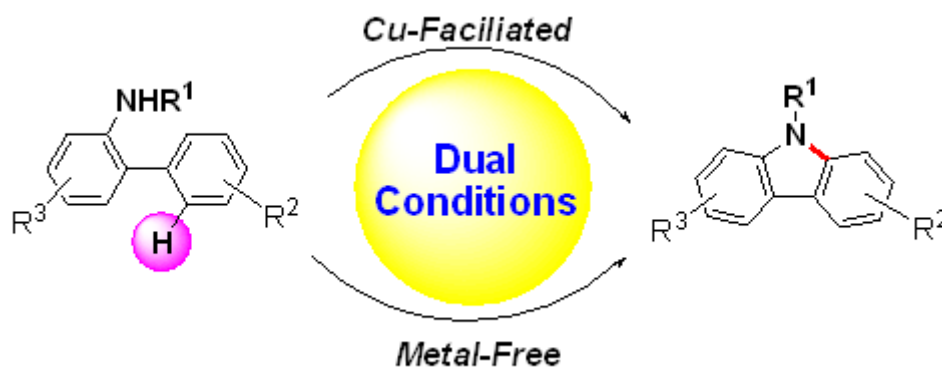
발표종류: 포스터, 발표일시: 목 15:00~17:00

## Intramolecular Oxidative C-N Bond Formation for the Synthesis of Carbazoles: Comparison of Reactivity between the Cu-Catalyzed and Metal-Free Conditions

조승환, 윤정호, 장석복

KAIST 화학과

New synthetic procedures of intramolecular oxidative C-N bond formation have been developed for the preparation of carbazoles starting from N-substituted amidobiphenyls under either copper-catalyzed or metal-free conditions using hypervalent iodine(III) as an oxidant. In this transformation, a combined use of copper(II) triflate and the iodine(III) species significantly improves the reaction efficiency, allowing a more diverse range of products to obtain in good to excellent yields.



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발표코드: II-ORGN.P-227

발표분야: 유기화학

발표종류: 포스터, 발표일시: 목 15:00~17:00

## Conversion of L-Amino acid to D-form by Naphthol-Based Aldehyde

이예정

이화여대 화학나노과학과

Amino acid is the most representative chiral material. In particular, D-amino acids are used in food technology and as drug intermediates in Pharmaceuticals. Nevertheless, compared to L-amino acids, these D-amino acids are not abundant in nature. Therefore, the synthesis of D-amino acids in an easy and cost-effective way is very important. Naphthol-Based Aldehyde can convert the L-amino acids to D-amino acids. Receptor is designed to enhance the stereoselectivity of existing Naphthol-Based Aldehyde as the movement between the naphthalene rings of the receptor is restricted by steric hindrance. Receptor reacts with L-amino acids in DMSO-d<sub>6</sub> to form imines. After the addition of TEA, and the time dependant of <sup>1</sup>H-NMR spectrum of the imines proves the conversion of the L-amino acids to D-amino acids, through decreasing the L-form imine peak and increasing the D-form imine peak.

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## **BF<sub>3</sub>·SiO<sub>2</sub> catalysed One-pot synthesis of poly functionalized Mannich bases**

**Someshwar, 정연태**

부경대 이미지시스템공학과

In this letter, we reported the use of silica-supported boron trifluoride (BF<sub>3</sub>·SiO<sub>2</sub>) for the promotion of modified one-pot Mannich condensation of ketones, aldehydes and ammonium acetate in 1:2:1 ratio to afford the 3,5-disubstituted-2,6-diarylpiperidin-4-ones in high yields. This simple, easily preparable and reusable versatile catalyst effected the condensation very efficiently in shorter duration than the conventional method. All the reactions yielded a stereospecific product with equatorial orientation of all substituents in the chair conformation.

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## **Synthesis, Characterization and electronic properties of perylene-conjugated oligomers-perylene triads for n-type material**

심보람, 이진국, \*도정윤

부산대 고분자공학과 \*부산대 화학교육과

Donor-acceptor molecules have been considered in applications such as light harvesting, photocatalysis and organic photovoltaic cells for energy conversion. We have attempted to develop series of novel perylene-conjugated oligomers-perylene triad systems. They comprised head-to-tail-coupled low band gap pi-conjugated oligomers integrated between two terminal perylene bay sites. Diels-Alder reaction was pre-performed with maleic anhydride and dienophile of designed perylene bisimide and then coupled with diamines for the triad system. Optical energy transferring property and electronic conduction will be discussed with UV, PL, CV, and XRD analysis according to the structure of donor segments.

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## Synthesis of isomers of bicycloalkane dinitrate and their cetane number improving property

hoang quoc viet, 이신호, 이병욱, 김영준

충남대 화학과

The series of bicyclic nitrate and carbonate derivatives were synthesized from norbornene and dicyclopentadiene. To investigate the correlation between cetane number improving properties and configuration of nitrate groups, they were added to diesel fuel and the cetane number was measured by ASTM method. The results showed that there were noticeable improvement of cetane numbers (2~4 for nitrate compounds, 0.1~0.2 for carbonate compounds). It also showed that trans-dinitrate isomer has higher cetane number than cis-dinitrate and mononitrate derivatives.

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발표종류: 포스터, 발표일시: 목 15:00~17:00

## Synthesis and X-ray crystal structure of some di-1,3,4-thiadiazole derivatives.

hoang quoc viet, 이병욱, 김영준

충남대 화학과

Two di-1,3,4-thiadiazole derivatives were synthesized. One is thionate using Lawesson's reagent and the other is the compound from the reaction of mercapto-1,3,4-thiadiazole and alkyl dibromide. They were recrystallized in ethanol to produce proper crystals for Single Crystal X-Ray Crystallography. We will discuss the crystal structures and their UV spectra.

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## Polycyclic thioketals for high refractive index and thermally stable optical polymer

김새미, \*도정윤

부산대 화학교육학과 \*부산대 화학교육과

Refractive index is expressed as a ratio of the speed of light in a vacuum relative to a speed through a given medium. It is an important physical property to qualify optical materials and an essential value for optical applications such as lenses, prisms, optical waveguide, laser and so on. The chief ingredients of many optical materials are inorganic matter such as silica and inorganic crystals. Unlike conventional hard inorganic optical materials, organic optical materials have many advantages such as lightness, flexibility, easy synthesis process. In spite of these advantages, they have application limit due to low refractive index. Refraction is based on the interaction of electrons in a molecule with the oscillating electronic field of light. Electron-rich atoms such as sulfur or bromine or iodine are known to result in high refraction. We have designed and investigated new molecular structures in assumption that higher sulfur content in a unit volume induces larger refractive index. In this report, we will suggest polycyclic molecules capable to carry many sulfur atoms as possible in a molecular volume. Cyclic thio-ketals are the best candidate to achieve these missions and introduced unrestrictedly into polycyclic molecules.

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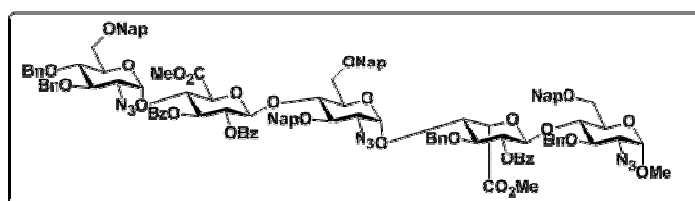
## Development of an Efficient Method for the Synthesis of Monosaccharide, Disaccharide, Trisaccharide and Pentasaccharide

이현숙, 김관수

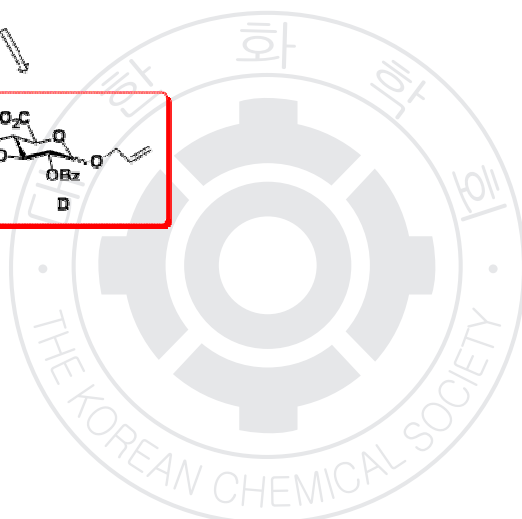
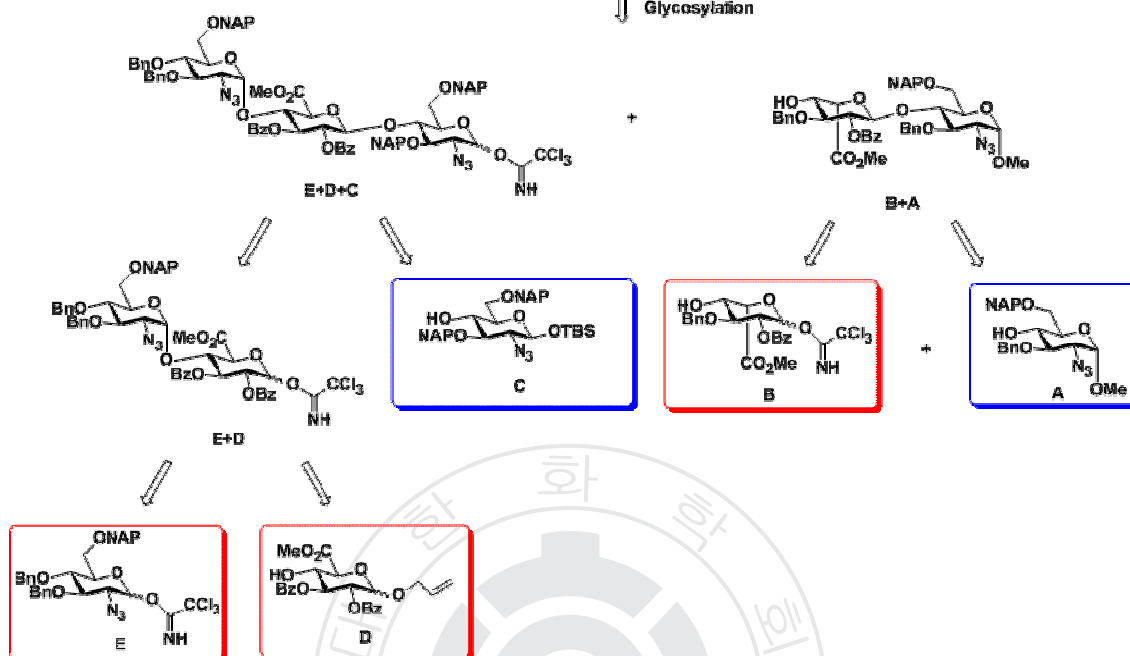
연세대 화학과

The object of this study is to develop an efficient method for the synthesis of five monosaccharide building blocks (A, B, C, D and E), two disaccharide units (A+B and D+E), a trisaccharide (C+D+E), and a Pentasaccharide(A+B+C+D+E). Glycosylation of the glycosyl acceptor A+B with the glycosyl imidate donor C+D+E employing TMSOTf as the promoter provided the target pentasaccharide stereoselectivity. Deprotection and selective sulfation are under progress.





Stereoselective  
Glycosylation



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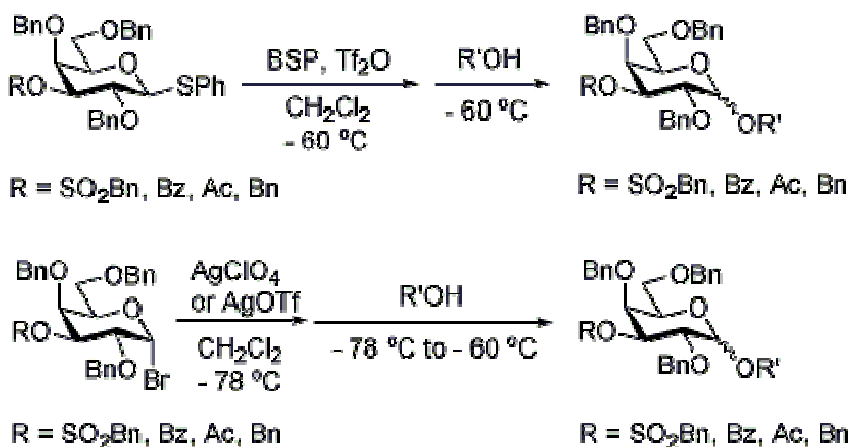
발표종류: 포스터, 발표일시: 목 15:00~17:00

## **$\alpha$ -Directing Effect in Glycosylations by Remote Participation of 3-O-Acyl Groups of Galactosyl Donors.**

명세진, 김관수

연세대 화학과

Previously, we reported the  $\beta$ -directing effect of electron-withdrawing groups at *O*-3, *O*-4, and *O*-6 positions and the  $\alpha$ -directing effect due to remote participation of 3-*O*-acyl and 6-*O*-acetyl groups of donors in mannosylations. Herein we report the  $\alpha$ -directing effect by remote participation of 3-*O*-acyl groups of galactose donors in galactosylations. Galactosyl donors possessing benzylsulfonyl, benzoyl, acetyl, and benzyl groups were prepared. The outcome of the stereochemistry in glycosylations of various acceptors with these donors indicated that 3-*O*-acyl groups of galactose donors participated during glycosylations. And a small amount of a bicyclic trichlorooxazining ring resulting from the intramolecular trapping of the anomeric oxocarbenium ion by 3-*O*-trichloroacetimidoyl group provided evidence for this remote participation. Also, we performed galactosylations of two glycosyl acceptors with galactosyl bromides, by employing either  $\text{AgClO}_4$  or  $\text{AgOTf}$  as the promoter, to examine the counteranion effect of the galactosyl oxocarbenium ion on the stereochemical outcome in the present galactosylations.



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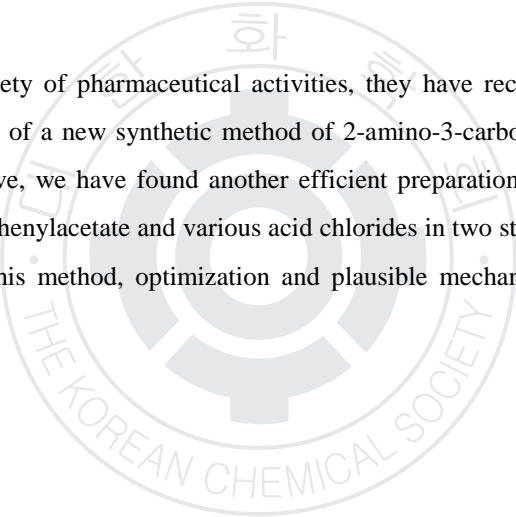
발표종류: 포스터, 발표일시: 목 15:00~17:00

## Efficient synthesis of benzofuran 3-carboxylic acids

이민형, \*김형백, 지대윤

서강대 화학과 \*서강대

As benzofurans have a variety of pharmaceutical activities, they have recieved a scientific attraction. Based on our recent finding of a new synthetic method of 2-amino-3-carboxamidobenzofurans from o-cyanomethylphenol derivative, we have found another efficient preparation of benzofuran 3-carboxylic acids from ethyl o-hydroxyphenylacetate and various acid chlorides in two steps with good overall yields. The logic of how to find this method, optimization and plausible mechanism of this method will be demonstrated.



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발표종류: 포스터, 발표일시: 목 15:00~17:00

## Biological Properties and Synthesis of Carboranyloximes as Potential BNCT Agents

이채호, \*박관희, \*조석준, \*\*이종대, \*\*\*강상욱

원광대 생명나노화학부 \*원광대 화학과 \*\*조선대 화학과 \*\*\*고려대 소재화학과

Carboranes are stable, lipophilic structures which resemble benzene in term of reactivity and bulkiness. Therefore it is not surprising that carborane-based biomolecules which an aromatic group is replaced by the boron cage have been prepared. Since carboranes which linked a biomolecule contain ten boron atoms, they theoretically may help deliver much higher concentrations of  $^{10}\text{B}$  atoms in cancer cells for boron neutron capture therapy (BNCT). Carboranylaryloximes containing water-soluble functional group have been synthesized and evaluated growth inhibition of various tumor cell lines and boron corporation into B-16 melanoma cell.

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발표종류: 포스터, 발표일시: 목 15:00~17:00

## Cobalt- and Manganese-Catalyzed Direct Amination of Azoles under Mild Reaction Conditions and the Mechanistic Details

김지영, 조승환, Jomy Kuruthukulangar, 장석복

KAIST 화학과

We have developed a new catalytic system for the direct amination of azoles with amines by using cobalt or manganese catalyst in the presence of peroxide and acid additive. The reaction is highly attractive from the synthetic point of view in that the catalyst loadings are low, optimal reaction conditions are mild, and substrate scope is broad. The present reaction, therefore, is anticipated to be a powerful tool for the synthesis of 2-aminoazoles which are an important pharmacophore of high biological activity. In addition, a mechanistic proposal is made on the basis of the kinetic isotope effects and isolation of amidine compounds.



*low catalyst loadings  
mild reaction conditions  
broad substrate scope*

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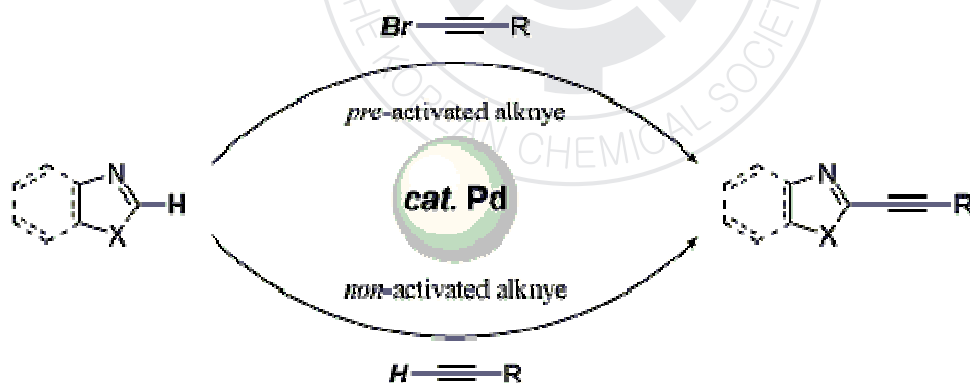
발표종류: 포스터, 발표일시: 목 15:00~17:00

## Palladium Catalyzed Alkynylation of Heterocycles using 1-Bromoalkynes and 1-Alkynes

김석환, 장석복

KAIST 화학과

Recently lots of couplings between 1-haloalkynes and various C-H bonds have been reported, although Sonogashira reaction has been applied as a powerful strategy for introducing sp carbon. Our group also found palladium catalyzed alkynylation of heterocycles using 1-bromoalkynes. Furthermore, we accomplished the employment of terminal alkynes for the alkynylation of azole type heterocycles.



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## Optically Transparent Sulfur-containing Alicyclic Polyurethane with High Refractive Index

이재은, \*김새미, \*\*도정윤

부산대 첨단정보및디스플레이소재협동과정 \*부산대 화학교육학과 \*\*부산대 화학교육과

Sulfur-containing alicyclic polyurethane was developed for low dispersion and high refractive index and characterizations were performed for convenient synthesis. Sulfur-containing high refractive index polymers have been developed in recent years for optoelectronic applications such as lenses, optical circuits, optical fibers, anti-reflective films and coatings, optical adhesives, waveguides, UV-reactive inks etc. In order to enhance the high refractive index, we synthesized sulfur containing alicyclic polyurethane successfully by radical reaction. As expected, sulfur attached polyurethane showed relatively high refractive index, low birefringence and better optical transparency. These urethane polymers are promising for optical applications such as optical switches, attenuator and splitter requiring high thermo-optic effect.

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## Asymmetric Synthesis of (R)-2-(2-chloroethyl)pyrrolidine-1-carboxylic acid ethyl ester

김희두

숙명여대 약학대학

In connection with our recent report on the stereoselective synthesis of H1 receptor antagonist clemastine, we present here the stereoselective synthesis of (R)-2-(2-chloroethyl)pyrrolidine-1-carboxylic acid ethyl ester for clemastine amine using stereoselective N-allylation and ring closing metathesis as key steps. The commercially available (S)-(-)- $\alpha$ -Amino- $\gamma$ -butyrolactone was treated with allyl bromide and LiI to give the corresponding N-diallylated butyrolactone in good yield. Selective removal of one allyl group with ethyl chloroformate gave the desired mono-N-allylated product in good yield. This two-step sequence permits us to minimize the racemization during the allylation process, and to get the product in high yield. Then, the mono-N-allylated butyrolactone was transformed to the requisite diene for ring closing metathesis in 2 steps via Dibal-H reduction and Horner-Wadsworth Emmons olefination. The diene was then subjected to RCM reaction using commercially available 2nd generation Grubbs' catalyst in dichloromethane to produce the 5-membered pyrrolidine in 90% yield. Subsequent hydrogenation, and followed by chlorination with Viehe salt produced (R)-2-(2-chloroethyl)pyrrolidine-1-carboxylic acid ethyl ester. In summary, we will present that optically active amine for clemastine can be prepared efficiently from our method using stereoselective N-allylation and ring closing metathesis.



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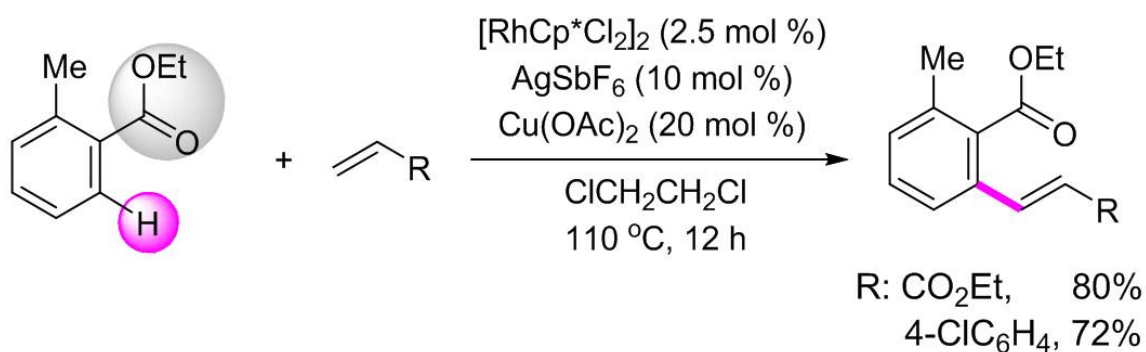
발표종류: 포스터, 발표일시: 목 15:00~17:00

## Rh(III)-Catalyzed Regioselective Olefination at the ortho-Position of Arene Esters via C-H Bond Activation

박세훈, 김지영, 장석복

KAIST 화학과

A new catalytic procedure of ortho-olefination of benzoates and benzaldehydes has been developed. Ester and carboxaldehyde unit were revealed to be effective chelating groups to direct the activation of aryl C-H bonds ortho to the directing moieties under the Rh-catalyzed oxidative conditions (see scheme). The reaction is highly regioselective with a range of benzoates and benzaldehydes enabling the efficient olefination with arylates, acrylic acid, and styrenes.



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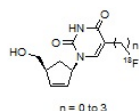
발표종류: 포스터, 발표일시: 목 15:00~17:00

## Synthesis of Carbocyclic 5-[<sup>18</sup>F]Fluoroalkylated Pyrimidine Nucleosides

안현석, \*안광일, 서정원, 이학준

한양대 응용화학과 \*한국원자력의학원 방사성의약품 개발실

Interest in the synthesis of carbocyclic nucleosides and carbocyclic analogues of normal nucleosides has grown exclusively since the potential antiviral and antitumor therapeutic agents. The replacement of the furanose oxygen by a carbon gives the nucleoside increased in vivo stability. carbocyclic nucleosides, 1-[4-(hydroxymethyl)-cyclopent-2-enyl]-5-[<sup>18</sup>F]fluoroalkyluracil analogues were synthesized via Pd(0)-catalyzed coupling reaction and radiofluorination as key reactions.



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## **Ionic Liquids Co-lyophilized Enzyme for Biocatalysis in Organic Solvent: Remarkedly Enhanced Activity and Enantioselectivity of Enzyme**

이재관, \*김도형, \*김혜선, \*이슬

호서대 그린에너지공학과&융합기술연구소 \*호서대 그린에너지공학과

Nonaqueous biocatalysis provide a useful component of methodology in organic synthesis. For example, lipase catalysis in organic solvents is of great use for the synthesis of optically active compounds such as chiral alcohols, acids, and their esters. However, biocatalysis in nonaqueous media often suffer from reduced activity, selectivity or stability of enzyme. The use of ionic liquids as an alternative solvent in the biotransformation proved the enhanced activity, selectivity, and stability of enzyme. The room temperature ionic liquids (RTILs) are very attractive materials. They are organic salts and their various properties, such as solubility in solvents, melting point, conductivity, and etc, are tunable. Particularly, the room temperature solid-phase ionic liquids (RTSPILs), which become liquids at elevated temperature, led us to envisage that they might be suitable as lyoprotectants for activation of biocatalyst by lyophilization, as well as coating materials. Herein, we present the results of the study on the RTSPILs co-lyophilized enzyme that exhibited markedly enhanced reactivity for biocatalysis in organic solvent showing around 66-fold and 660-fold better catalytic activity compared with the crude and salt-free lyophilized enzyme, respectively. We observed that the enhanced activities by RTSPILs were mainly attributable to the size affection of enzyme catalyst after co-lyophilization with RTSPIL. Also, the enantioselectivity of RTSPIL co-lyophilized enzyme showed 2.5-fold more enhanced enantioselectivity than crude and salt-free lyophilized enzyme.

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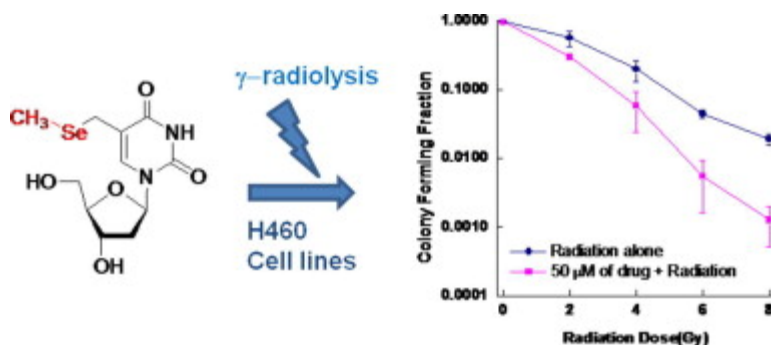
발표종류: 포스터, 발표일시: 목 15:00~17:00

## Potent radiosensitizing agents: 5-Methylselenenyl- and 5-phenylselenenyl-methyl-2'-deoxyuridine

Ambadas B. Rode, 홍인석

공주대 화학과

We developed novel radiosensitizing agents in vitro based on nucleoside base modification. In addition to the known 5-phenylselenide derivative, 5-methylselenide modified thymidine, which has a van der Waals radius smaller than the phenyl group, was newly synthesized. The similar monomer activity of 5-methylselenide derivative under oxidation condition was confirmed by NMR experiments. The cytotoxicity tests and radiosensitizing experiments of both compounds were carried out using the H460 lung cancer cell line. Both the 5-phenylselenide and the 5-methylselenide derivatives showed a relatively low toxicity to the cells. However, in combination with  $\gamma$ -radiolysis, both exerted good radiosensitizing effects to the lung cancer cell lines in vitro. This result confirms that 5-methylselenide modified thymidine could be a useful candidate as a potential radiosensitizing agent in vivo.



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발표종류: 포스터, 발표일시: 목 15:00~17:00

## Mixing Magnesium and Engineering Plastic (PC) adhesive for Mobile use and its Evaluation

이준균

한국생산기술연구원 열표면기술연구부

As a result of analyzing existing urethane-epoxy copolymer resin for designing adhesive base resin, the use of a mix of polymers with different molecular weights was confirmed to produce an adhesive with better performance than normal. In this study, for the purposes of developing a high-performance adhesive, we studied mobile-use magnesium and engineering plastic adhesive by optimizing the mix ratio of base polymer and secondary adhesive for property improvement. By evaluating a synthetic resin based on the above, we analyzed chemical micro-structure of the main adhesive, the morphological characteristics and crystallization of base polymer, aggregation, melting temperature, etc. Ultimately, by blending a main adhesive PU and secondary adhesives SEBS and NBR, we synthesized a superior base polymer with 300% elongation and 6.5MPa adhesive strength.

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발표분야: 유기화학

발표종류: 포스터, 발표일시: 목 15:00~17:00

## Chirality Converting Reagent Based on Binol Aldehyde Pendant with Linear-chained Guanidinium

조예슬

이화여대 화학나노과학과

Optically pure D-amino acids are useful intermediates as synthesis of pharmaceuticals and food ingredients. In the past years, we designed and synthesized novel binol based chiral receptors for amino acids and amino alcohols called as ARCA(Alanine Racemase Chiral Analogue) systems. These receptors have good selectivity for amino alcohols and can convert L-amino acids to D-amino acids. These receptors make reversible imine bond with amino alcohols which have the advantage of being much stronger and structurally well defined compared to the noncovalent interactions. Besides the imine bond, a resonance assisted hydrogen bond(RAHB) and other hydrogen bonds between the acid/alcohol group and the receptor play important roles in determining the stereoselectivity. We constantly report here a novel ARCA receptor which has many advantages such as solubility in organic solvents and high enantioselectivity towards the chiral amino acids and amino alcohols, compared to the other developed receptors. Guanidinium based chiral receptor has been designed, the synthetic details of receptors and the recognition properties will be presented.

일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: II-ORGN.P-247

발표분야: 유기화학

발표종류: 포스터, 발표일시: 목 15:00~17:00

## Synthesis and evaluation of antitumor activities of new lead compounds of Hanultarin.

이은영, V.S.Jamal Ahamed, Mahto Sanjeev Kumar, 이석우, 문석식, 홍인석

공주대 화학과

Previously, we showed that the isolated Hanultarin from *Trichosanthes* seed has a good antitumor activity. In this study, seven derivatives of Hanultarin were first synthesized and their structures were confirmed by spectroscopic methods such as IR, NMR, Mass. Cytotoxicities of these derivatives were evaluated by SRB assay using B16F10, HCT-15, A549, SKOV3 and SKMe12 cell lines respectively. At least four compounds showed similar  $IC_{50}$  values to that of cisplatin ( $\sim 10$   $\mu\text{g/mL}$ ). Furthermore, Immunofluorescence analysis was carried out to check effects on the intracellular structures such as actin and microtubules cytoskeleton using A549 cell line. In contrast to Hanultarin, these derivatives caused disruption of both actin and microtubules in A549 cell.

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장소: 제주ICC

발표코드: II-ORGN.P-248

발표분야: 유기화학

발표종류: 포스터, 발표일시: 목 15:00~17:00

## Correlation of the Rates of Solvolysis of 1-Peperidincarbonyl chloride Using the Extended Grunwald-Winstein Equation

최호준, \*구인선

경상대 화학과 \*경상대 화학교육과

The specific rates of solvolysis of 1-peperidincarbonyl chloride (1) have been determined in 26 pure and binary solvents at 25.0 °C. In most solvents the values are essentially identical to those for 4-morpholinecarbonyl chloride. Linear free energy relationship (LFER) comparison of the specific rates of solvolyses of 1 with those for p-methoxybenzoyl chloride and those for 4-morpholinecarbonyl chloride are helpful in the mechanistic considerations, as is also the treatment in terms of extended Grunwald-Winstein equation. It is proposed that the solvolyses of 1 in the binary aqueous solvent mixtures proceed through ionization [I] pathway channels rather than through an  $S_N1/S_N2$  and/or ionization/(ionization-elimination)=[I/(I-E)] pathway channels.



일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: II-ORGN.P-249

발표분야: 유기화학

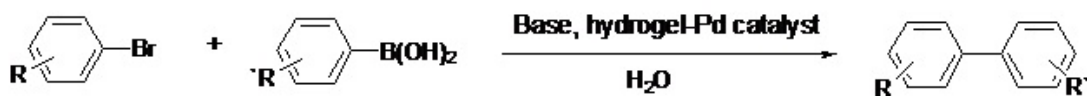
발표종류: 포스터, 발표일시: 목 15:00~17:00

## Preparation of thermo-responsive hydrogels as solid-support of Pd nanoparticles and their application in Suzuki-Miyaura cross-coupling reaction

홍명찬, \*이종복, 이학준

한양대 응용화학과 \*한양대 바이오테크놀로지학과

Temperature-responsive hydrogels which exhibit phase transition at a lower critical solution temperature (LCST) are well-studied. Below the LCST, a hydrogel incorporates water and swells whereas it releases water above the LCST and shrinks. Poly(N-isopropylacrylamide-co-4-vinylpyridine) [poly-NIPAM-co-4-VP] copolymer microgels which have inverse temperature solubility and LCST in water have been synthesized using varying contents of 4-vinylpyridine. We prepared Pd(0) catalyst using poly-NIPAM-co-4-VP as a supporting material. We have developed an efficient and green heterogeneous Pd(0) nano catalyst system for Suzuki-Miyaura cross-coupling reaction in water.



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장소: 제주ICC

발표코드: II-ORGN.P-250

발표분야: 유기화학

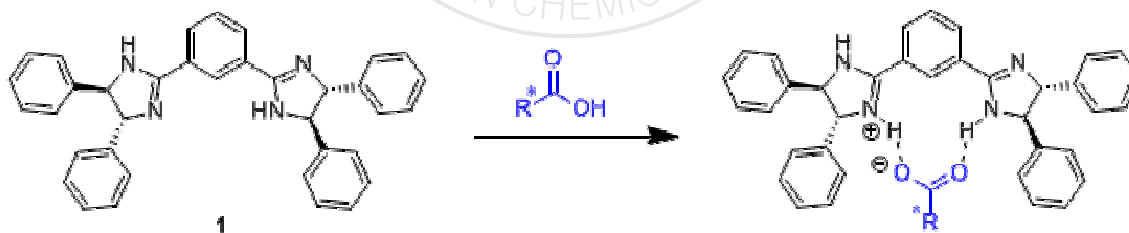
발표종류: 포스터, 발표일시: 목 15:00~17:00

## A Bisimidazoline Compound for the Chiral NMR Discrimination of Carboxylic Acids

김선미, 최기향

고려대 화학과

A new chiral solvating agent, 1,3-bis(imidazolin-2-yl)benzene (1), has been prepared from isophthalaldehyde and (*S,S*)-1,2-diphenylethylenediamine through a single step synthesis. This agent can bind with carboxylic acids through hydrogen bonding and, in the presence of one equivalent of 1, two enantiomers of a chiral carboxylic acid show different  $^1\text{H}$  NMR chemical shift values. This chemical shift nonequivalence is generally large enough so that the enantiomeric purity of the carboxylic acid could be easily determined. Studies with related compounds showed that the 1,3-disubstituted structure is crucial for the acid binding and chiral discrimination ability of 1.



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장소: 제주ICC

발표코드: II-ORGN.P-251

발표분야: 유기화학

발표종류: 포스터, 발표일시: 목 15:00~17:00

## Synthesis of Dendrimers via Sonogashira Coupling Reaction

이재욱, 박다정, 한승철

동아대 화학과

A coupling reaction in organic chemistry is a catch-all for a range of reactions in organometallic chemistry where two hydrocarbon fragments are coupled with the aid of a metal catalyst supported by suitable ligands. A Sonogashira reaction (palladium and copper co-catalyzed coupling of terminal alkynes with aryl and vinyl halides) is one of the most widely used C-C bond-forming reactions in organic and material chemistry. We will investigate the Sonogashira coupling reaction for the synthesis of Fréchet-type dendrimers from the alkyne focal point functionalized Fréchet dendrons and 1,4-diiodobenzene.

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장소: 제주ICC

발표코드: II-ORGN.P-252

발표분야: 유기화학

발표종류: 포스터, 발표일시: 목 15:00~17:00

## Synthesis of Symmetric Fréchet-type Dendrimers Using Homo-coupling of Terminal Alkyne

이재욱, 송태균, 한승철

동아대 화학과

The homocoupling of terminal alkynes is a straightforward method for the synthesis of buta-1,3-diynes, 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 homocoupling of terminal alkynes, this method has attracted a great deal of interest due to its mildness and wide-ranging substituent tolerance. Taking advantage of these facts, herein we will present the efficient strategy for the convergent synthesis of emissive Fréchet-type dendrimers containing a chromophore from alkyne focal point functionalized Fréchet-type dendrons via homo-coupling reaction of terminal alkyne which may be a kind of new click chemistry.

일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: II-ORGN.P-253

발표분야: 유기화학

발표종류: 포스터, 발표일시: 목 15:00~17:00

## Synthesis and Characterization of Fréchet-type Dendrimers Using Staudinger/aza-Wittig Reactions

이재욱, 곽승환, 한승철

동아대 화학과

The click chemistry is a modular approach that uses the most practical and reliable chemical transformations and has found in many applications in organic chemistry and synthesis of polymer and dendrimer. Staudinger/aza-Wittig reactions are also a powerful tool in organic synthetic strategies directed towards the construction of nitrogen-containing compounds. Taking advantage of these facts, herein we will disclose the general and efficient strategy for the convergent synthesis of various Fréchet-type poly(arylether) dendrimers containing via Staudinger/aza-Wittig reactions (new click reaction) between azide and aldehyde. Our strategies are in situ Staudinger/aza-Wittig reactions using an azido group and aldehyde in the presence of triphenylphosphine and followed by the reduction of imine intermediates.

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장소: 제주ICC

발표코드: II-ORGN.P-254

발표분야: 유기화학

발표종류: 포스터, 발표일시: 목 15:00~17:00

## Fluorous and Fluorescent Tag System for Chemical Array

강명구, \*김민혜, 박균하, \*전문국

충남대 화학과 \*한국화학연구원 대사증후군치료제연구센터

Chemical array is defined as a solid surface on which a spatially addressable and high-density array of small organic compounds is introduced. During about the past decade, it has attracted much attention as a potential format for detection of small organic partners bound to various protein targets in a high throughput manner, which could provide chemical tools for study on biological phenomena and/or new drug research through secondary multidimensional evaluation process. The technology is comprised of key elements such as design and synthesis of a small molecule library, immobilization of the library molecules to chemically modified surfaces, detection of small molecule-protein interactions, and data analysis. In this presentation, we would like to report a fluorous and fluorescent tag system for tagging of small organic compounds, their immobilization, and monitoring of their immobilization behavior, which could facilitate the quality control of small molecule microarray fabrication process. Design and synthesis of the tag system will be described together with preliminary results from proof-of-concept microarray experiments.

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장소: 제주ICC

발표코드: II-ORGN.P-255

발표분야: 유기화학

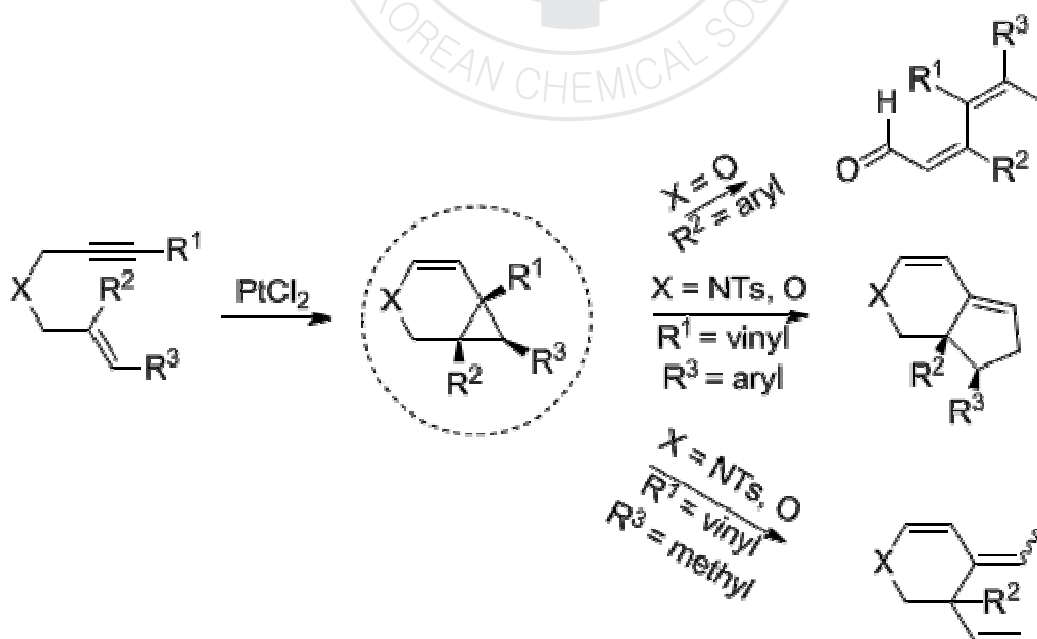
발표종류: 포스터, 발표일시: 목 15:00~17:00

## Tandem Platinum Dichloride-Catalysis and Rearrangement of Enynes: Versatile Synthetic Platform Based on Bicyclo[4.1.0]hept-2-enes

손소리, \*정영근

서울대 자연과학대학 화학부 \*서울대 화학부

A tandem PtCl<sub>2</sub>-catalyzed cycloisomerization and rearrangement reaction of enynes led to the formation of 2,4-pentadienals, 1-aryl-tetrahydro-1H-indenes, or 3-methylene-4-vinylcyclohex-1-enes; depending upon the substituent(s) and tether group of the enynes, the PtCl<sub>2</sub>-catalyzed cycloisomerization products, bicyclo[4.1.0]hept-2-enes, undergo a Claisen rearrangement, a 1,5-hydrogen shift, or a vinylcyclopropane rearrangement.



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장소: 제주ICC

발표코드: II-ORGN.P-256

발표분야: 유기화학

발표종류: 포스터, 발표일시: 목 15:00~17:00

## The effect of intramolecular charge transfer via biphenyl group on the optoelectronic properties of red fluorophore

박나래

홍익대 화학공학과

A new red fluorescent material, (2Z,2'Z)-3,3'-[4,4''-bis(dimethylamino)-1,1':4',1''-terphenyl-2',5'-diyl]bis[2-(pentafluorophenyl)acrylonitrile] (ABCV-PFP) for organic light-emitting diodes (OLEDs) was synthesized. To verify the effect of intramolecular charge transfer (ICT), UV-visible absorption and photoluminescence (PL) emission spectra of ABCV-PFP were measured with the variation of solvent polarity (n-hexane, n-hexane/chloroform = 1/1; chloroform; methylene chloride). The absorption peaks of ABCV-PFP were measured to be 330 (methylene chloride), 331 (chloroform), 328 (n-hexane/chloroform = 1/1) and 323 nm (n-hexane), respectively. PL emission spectra of ABCV-PFP were peaked at 645 (methylene chloride), 639 (chloroform), 609 (n-hexane/chloroform = 1/1) and 556 nm (n-hexane), respectively. UV-visible and PL emission spectra measured in various solvents showed large Stokes shifts. The UV-visible absorption maxima of ABCV-PFP showed small red shifts with increasing solvent polarity. This can be interpreted as that dipolemoment of the ABCV-PFP molecule in ground state is very small. Unlike the UV-visible absorption spectra, PL emission spectra showed strong solvatochromic red shifts with increasing solvent polarity. Strong positive solvatochromism of PL emission spectra of ABCV-PFP supported that ABCV-PFP molecule has a large molecular dipolemoment in its excited state which is ascribed to the molecular structure of ABCV-PFP in excited state caused by ICT between electron donating dimethylamino group attached to the biphenyl group and electron accepting moiety in the molecule.



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장소: 제주ICC

발표코드: II-ORGN.P-257

발표분야: 유기화학

발표종류: 포스터, 발표일시: 목 15:00~17:00

## Chromatographic separation, absolute structure determination and evaluation of herbicidal activities of new chiral isoxazoline derivatives

남준호, \*고영관, \*\*연구환, \*류재욱, \*구동완, \*\*\*조창우

경북대 화학과, 한국화학연구원 \*한국화학연구원 바이오소재연구센터 \*\*한국화학연구원 화학  
물질연구단 \*\*\*경북대 화학과

5-(2,6-Difluorobenzyl)oxymethyl-5-methyl-3-(3-methylthiophen-2-yl)-1,2-isoxazoline (Methiozoline), which is commercialized as a turf herbicide in Moghu Research Center, 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. Field trials indicated that this compound controlled annual weeds rapidly with a good tolerance on transplanted grass seedlings by postemergence and soil application. This compound showed a low mammalian and environmental toxicity in various toxicological tests. However, this compound has the racemic configuration. After chiral separation of the intermediates followed by coupling reaction, we could isolate the optical isomers of Methiozoline derivatives. We could also determine the absolute structures employing X-ray crystallography. Greenhouse experiments for the optical isomers showed that the isomers having S configuration are active and the isomers having R configuration are inactive.

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장소: 제주ICC

발표코드: II-ORGN.P-258

발표분야: 유기화학

발표종류: 포스터, 발표일시: 목 15:00~17:00

## Ground- and Excited-State Intermolecular Interactions in Supramolecules-Embedded Polymer System

김종현, 윤성준, 박수영

서울대 재료공학부

Electron-donor (D)와 electron-acceptor (A) 간의 효과적인 에너지 레벨 조절 및 매칭은 p-n junction 을 필요로 하는 다양한 광전자 소자의 개발에 있어 필수적으로 요구된다. 본 연구에서는 서로 다른 분자 에너지 레벨을 갖는 electron-acceptor 인 초분자체들을 electron-donor 인 반도체성 고분자들에 도핑하여, 이들의 에너지 레벨에 따라 ground- 및 excited-state 에서 발생하는 다양한 분자간 상호작용 (ground-state charge-transfer complex (CTC), exciplex 형성, 그리고 electron-transfer 현상)과 이들이 나타내는 독특한 광전기적 특성에 대해 관찰하였다. 이러한 결과들을 바탕으로, 본 발표에서는 CTC 형성에 의한 유기물의 우수한 전기 전도도 구현, exciplex 가 형성되는 정도를 조절함으로써 다양한 파장대의 형광 제어, 그리고 exciplex 를 구성하는 초분자체들의 우수한 자기 조립력에 바탕을 둔 용매와 온도 감지 법에 대해 다루고자 한다. 또한 유기 태양광 전지 구동에 주요 메커니즘이 되는 electron-transfer 현상이 효과적으로 일어나기에 적합한 에너지 레벨 차이를 광전기적 분석을 통하여 밝혔다.

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장소: 제주ICC

발표코드: II-ORGN.P-259

발표분야: 유기화학

발표종류: 포스터, 발표일시: 목 15:00~17:00

## Highly Fluorescent Mechanochromic Crystals: Material Design, their Polymorphism, and Secondary Bonding Interaction in Molecular Stacking Assembly

윤성준, 박수영

서울대 재료공학부

최근  $\pi$ -공액 유기물의 고체 상태에서의 유기광전자 소자로의 적용이 이루어지고 연구 개발이 활발하게 진행됨에 따라, 고체상태에서의 분자의 적층 배열에 관한 집중적인 연구가 필요하게 되었다. 특히  $\pi$ - $\pi$  적층, 수소결합, C-H $\cdots$  $\pi$  상호작용, 쌍극자 상호작용과 같은 분자 적층을 제어할 수 있는 이차적인 분자간 상호작용에 관한 연구가 분자 공학 분야에서 활발하게 이루어지고 있다. 또한, 합리적인 분자구조 설계에 의한 분자간 상호작용의 조절은 기능성 분자 소재의 광전기적 특성을 제어하는 중요한 접근법으로 주목받고 있다. 본 연구실에서는 최근, 강한 극성을 갖는 한 쌍의 cyano 그룹을 distyrylbenzene 분자 구조에 도입하여 분자 적층 공학 기술의 개발을 진행하고 있다. Dicyanodistyrylbenzene 유도체들은 C-H $\cdots$ N 수소결합, C-H $\cdots$  $\pi$  상호작용, 쌍극자 상호작용이 동시에 작용하는 다중 2 차 결합력에 의해 규칙적인 초분자적 적층 구조체를 형성하게 된다. 이러한 분자 결정들은 두 가지의 다른 쌍극자 결합 구조 (antiparallel/head-to-tail 결합)와 재형성 가능한 2 차 결합 상호작용에 의해 유도되는 독특한 압력 변색성 형광 변화 특성을 보인다. 이 발표에서는 강한 고체상 형광과 함께 압력 변색성 형광 변화 특성을 보이는 새롭게 개발된 dicyanodistyrylbenzene 유도체 (2Z,2'Z)-2,2'-(1,4-phenylene)bis(3-phenylacrylonitrile) (BDCS) 와 (2Z,2'Z)-2,2'-(1,4-phenylene)bis(3-(naphthalen-2-yl)acrylonitrile) (NDCS)의 분자 설계, 다형결정성, 분자 적층 구조에서의 2 차 결합 상호작용의 역할에 대해 논의하고자 한다. 각각의 분자들로부터 두 가지의 다른 다형결정들을 제작할 수 있었고, 구조-특성 상관 관계와 압력 변색성 변형의 메커니즘에 대해 구조적, 광학적, 광물리적 접근법을 통하여 체계적으로 분석하였다. 이러한 소재들은 향후 새로운 압력 센서나 가역적인 광/정보 저장매체의 개발에 유용하게 적용될 수 있을 것으로 기대된다.

일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: II-ORGN.P-260

발표분야: 유기화학

발표종류: 포스터, 발표일시: 목 15:00~17:00

## Synthesis and Characterization of Quaterrylene Bisimide Colorants

박근수, 정연태

부경대 이미지시스템공학과

Near-infrared (NIR) colorants has special properties to collect light in the NIR wavelength region. Owing to this properties, NIR colorants are used in many industries, including in optical recording, NIR filter, NIR photography and solar cell. Among them, Quaterrylene colorants have the polycyclic aromatic structure. This structure is formed by many double bond, and usually exhibit excellent chemical stability and photo-stability because  $\pi$ -conjugation of polycyclic aromatic structure can make more strong strength. However, there are only capable of capturing the UV and visible light. Hence, in this study, we have kept the good properties of Quaterrylene colorants and then attached imide functional group on their surface. It affects the shift of the absorption band into NIR region. We have synthesized quaterrylene bisimide colorants from perylene derivatives via Suzuki coupling. Quaterrylene bisimide colorants properties were analyzed by Maldi-tof mass, TGA, Overlay spectrum, Elemental Analyzer, Chemical stability. Their properties showed absorption band at 700nm region (include to NIR region) and exhibit excellent chemical stability and photo-stability.

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발표종류: 포스터, 발표일시: 목 15:00~17:00

## Fabrication of High Performance Single Crystalline Organic Field-Effect Transistors via Solvent Annealing Technique

박상규, 김종현, 윤성준, 박수영

서울대 재료공학부

높은 결정성을 가지는 n 형 유기물 반도체 물질인 (2Z,2'Z)-3,3'-(1,4-phenylene)bis(2-(3,5-bis(trifluoromethyl)phenyl)acrylonitrile) (CN-TFPA)는 박막 및 결정상에서 독특한 광전기적인 거동을 나타낸다. 용액 공정을 통해 손쉽게 결정 성장이 가능한 CN-TFPA 분자는 두 가지의 서로 다른 분자 배열을 갖는 polymorphism (G-phase, B-phase) 현상 및 이에 따른 서로 다른 트랜지스터 특성을 나타내는데 이러한 현상은 반도체성 유기 단분자 반도체 물질의 핵심 연구 분야인 분자 배열에 따른 전기적 특성 평가에 대한 연구를 가능케 한다. 본 발표에서는 G-phase 와 B-phase 로 존재하는 CN-TFPA 의 서로 다른 분자 배열 구조 및 이에 따른 독특한 트랜지스터 특성, 그리고 비전통적인 결정 성장 법인 solvent vapor annealing (SVA) 법을 도입하여 제작된 우수한 결정 트랜지스터의 특성에 대해 발표하고자 한다.

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발표종류: 포스터, 발표일시: 목 15:00~17:00

## Synthesis and Properties of Highly Fluorescent Self-assembled Supramolecules with Multiple Hydrogen Bonds

김상훈, 윤성준, 박수영

서울대 재료공학부

$\pi$ -공액 유기물의 광·전기적 특성은 단위분자가 초분자 구조체를 형성하면서 변화한다. 따라서 초분자 구조체의 제어를 통한 유기물의 광·전기적 특성 조절에 대한 연구는 학술적, 응용적 측면에서 중요한 의미를 갖는다. 자기 조립에 의한 초분자 구조체는 분자간의 비공유 결합으로 유도되어 형성되는데, 수소결합은 이러한 이차적인 상호작용 가운데 선택성과 방향성이 뛰어나 분자 적층을 정확히 제어할 수 있다. 특히 다중수소결합을 이용할 경우 이중분자간의 자가분류(self-sorting)를 통한 복합 초분자 구조체를 만들 수 있을 뿐만 아니라, 초분자 구조체의 구조와 물성에 관한 예측과 제어가 용이하며, 2 차적인 특성 또한 기대할 수 있다. 본 그룹에서는 집합체 유도에 의한 형광 증진 현상을 보이며 삼중수소결합이 가능한 새롭게 개발된 시아노-스틸벤의 유도체인 (E)-N,N'-(4-(4-(2-(3',5'-bis(trifluoromethyl)biphenyl-4-yl)-1-cyanovinyl)phenyl)pyridine-2,6-diyl)diacetamide 을 합성하였다. 이 분자는 Cyanuric Acid 유도체와의 삼중수소결합을 통해 정렬된 초분자 복합체를 형성하였다. 그리고 이러한 구조체의 형성으로 발생한 광학적인 특성 변화를 관찰하였다. 본 발표에서는 위 분자의 다중수소결합 형태에 따라 변하는 초분자의 구조와 광학적 특성에 관해 보고하고자 한다.

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## Spontaneous Nanobelt Formation of a Designed Small Organic Molecule with Self-Complementarity

전아람, 정윤철, 이희승

KAIST 화학과

Biomolecular self-assembly is a powerful tool for constructing nano-/microscale complex functional systems, in which monomeric units are associated spontaneously by the combination of noncovalent interactions. Although dipeptide(FF) is known as the simplest building blocks providing self-assembled nanostructures in the literature, we wondered if it is possible to get a self-assembled structure from an amino acid level building block. In this presentation, we report an interesting result from our laboratory that a rationally designed unnatural amino acid was spontaneously assembled to form nanobelt structure in organic solvent. The key functional groups installed in the compound are identical to those in a well-known  $\beta$ -strand forming peptide, in which hydrophobic phenyl group and hydrophilic functionalities (ammonium and carboxylate) are positioned in alternative fashion.

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## Unprecedented Molecular Architectures by the Controlled Self-Assembly of $\beta$ -Peptide Foldamer

권선별, 공진택, 이희승

KAIST 화학과

During past decades, several types of peptide-based scaffolds, ranging from simple aromatic dipeptide to small protein fragments, have been studied to understand the underlying mechanism and mimic to create artificial nano/microstructures. However, a limited number of design principles have still been reported in peptidic scaffolds allowing well-defined self-assembled structure formation, presumably due to the intrinsic large conformational flexibility of natural peptides. In this presentation, we report the first example of highly homogeneous, well-defined and finite architectures by the  $\beta$ -peptide self-assembly.



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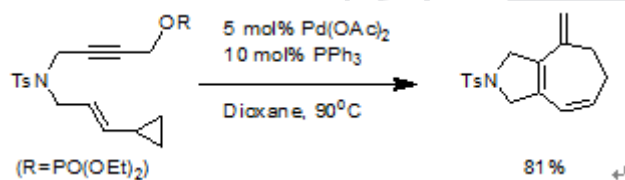
발표종류: 포스터, 발표일시: 목 15:00~17:00

## Palladium Catalyzed Cyclization of Cyclopropyl Enynes Bearing Phosphate or Methoxy Group

오혜미, 정영근

서울대 화학부

A palladium-catalyzed carbocyclization of cyclopropyl enynes has been studied. When enynes having phosphate were used as a substrate, 5,7-bicyclic compounds were isolated in reasonable to high yields. In case of enynes bearing methoxy group, 1-(buta-1,3-dienyl)-2-(methoxymethylene)cyclopentanes were isolated in reasonable yields. Depending upon the substituent on the propargyl group, different reaction products were isolated as a major product. The different reactivity will be discussed in detail.



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발표종류: 포스터, 발표일시: 목 15:00~17:00

## Construction of high-dimensional dendrimers by the axial coordination of pyridine-cored dendron on zinc porphyrin-cored dendrimers

최고은, 신은주

순천대 화학과

Porphyrin and metalloporphyrins are attractive molecular components for the purpose because of their unique structures and rich photoelectronic properties. A variety of dendrimers have been studied for their structural uniqueness to allow feasible molecular design and well-defined array. Construction of high-dimensional dendrimer may be possible by the formation of coordination complex between dendrimers of different type, such as coordination of pyridine-cored dendron on zinc porphyrin-cored dendrimer. Zinc porphyrin-cored dendrimers could form the coordination complexes with pyridine-cored dendron via axial ligation. This study shows the construction of high-dimensional porphyrin dendrimers by the axial coordination of pyridine-cored dendron on zinc porphyrin-cored dendrimer and the influence of the dendritic environments.

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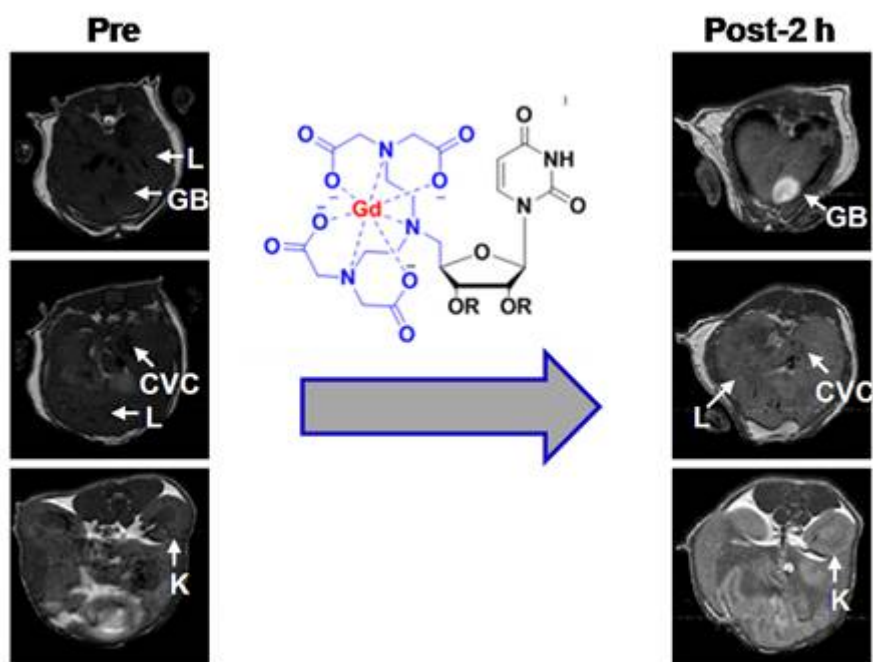
발표종류: 포스터, 발표일시: 목 15:00~17:00

## Uridine-based Paramagnetic Supramolecular Nanoaggregate: a Liver Specific T1 MRI Contrast Agent with High Relaxivity and pH Sensitivity

이수민, 김종승

고려대 화학과

we have synthesized uridine nucleoside-based amphiphilic gadolinium complexes as MRI contrast agents. The highest relaxivities achieved were 30.3 and 23.4 mM<sup>-1</sup>s<sup>-1</sup> in PBS (pH 7.4) at 0.47 and 1.41 T, respectively. The new complexes demonstrated binding affinity towards HSA with further enhanced relaxivity. Moreover, the relaxivity of amphiphilic contrast agents was changed depending on the pH of solution. The stability studies of the complexes against transmetallization with Zn<sup>2+</sup> indicated that these new amphiphilic complexes are quite stable and comparable with clinically used Gd-DTPA and Gd-DTPA-BMA. In vivo pharmacokinetics of the novel complex showed that the complex is highly specific for hepatocytes causing excretion into bile ducts, gall bladder, and intestines, and therefore it may be a highly potential T1 contrast agent to provide with detection of small lesions in liver. This contrast agent is first example of a self-assembled paramagnetic amphiphile with high relaxivity, significant binding ability with HSA, pH response, and high liver specificity among other reported amphiphilic gadolinium-based contrast agents. These new uridine-based amphiphilic contrast agents represent an important and highly efficient nanosystem for MRI applications.



L, liver; GB, gall bladder; CVC, caudal vena cava; K, kidney



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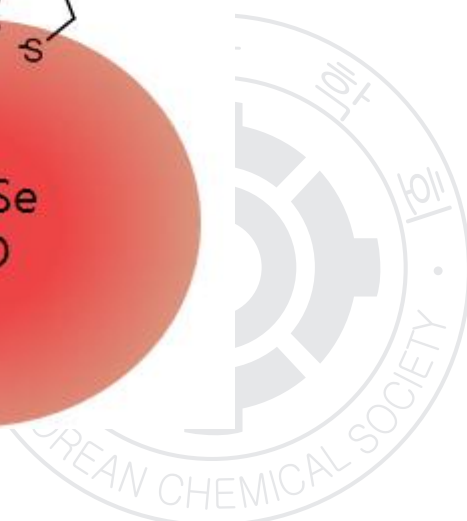
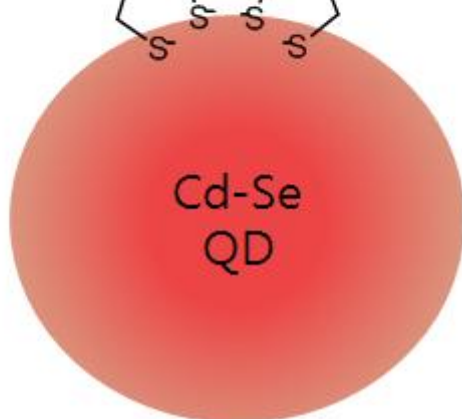
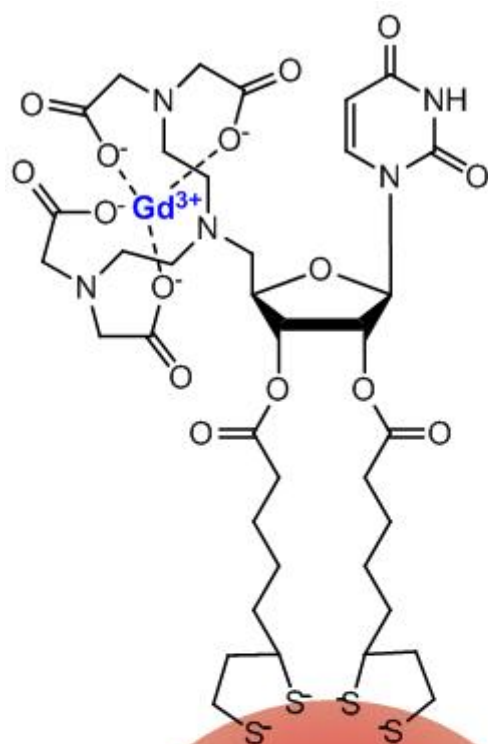
발표종류: 포스터, 발표일시: 목 15:00~17:00

## Uridine-based Nano Assembly: A liver directing bimodal contrast agent

박준원, 김종승

고려대 화학과

In recent years, magnetic resonance imaging(MRI) is one of the most widely used imaging modalities that provides high quality three dimensional images of tissues with anatomical informations. Also, semiconductor nanoparticles(quantum dots, QDs) have been used as fluorescence probes for cell labeling in optical imaging because of their high brightness, long-term photostability and single-light source excitation for multi-colored QDs. As reported that in pre-clinical studies multimodal contrast agent has been very effective for faster and more accurate prognosis that encourage us to design uridine-based fluorescent contrast agent. In connection with that we have synthesized water soluble uridine-based paramagnetic molecules binding with Cd-Se QDs. It has been characterized in regard to their  $T_1$  MRI contrast agent (CA) properties and fluorescence imaging agent.



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발표종류: 포스터, 발표일시: 목 15:00~17:00

## Establishment of the Mechanism of Conversion of 4-Hydroxybenzaldehyde into Picric Acid using Mass Spectrometry

박성훈, 이은화, 윤성화

아주대 분자과학기술학과

A novel, one-pot method for synthesizing picric acid (2,4,6-trinitrophenol) was previously reported by our group, in which the 4-hydroxyphenylglycine was converted to picric acid in a HNO<sub>3</sub>/H<sub>2</sub>O system via the formation of 4-hydroxybenzaldehyde. Although the mechanism for the conversion of 4-hydroxyphenylglycine to 4-hydroxybenzaldehyde was reported in the literature, the formation process of picric acid from 4-hydroxybenzaldehyde remained unclear. In order to establish the reaction mechanism of the formation of picric acid from 4-hydroxybenzaldehyde in the HNO<sub>3</sub>/H<sub>2</sub>O system, the same reaction condition was applied to 4-hydroxybenzaldehyde and 4-hydroxybenzoic acid, and the resulting intermediates were identified from each reaction. Intermediates were detected by electrospray ionization mass spectrometry (ESI-MS), and compared with authentic samples. The mass spectra of each reaction and the detailed procedure will be discussed.

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## Molecular Architectures by the Controlled Self-Assembly of a $\beta/\alpha$ -Foldamer

윤은영, 유성현, 이희승

KAIST 화학과

Recent advances in nanoscience have attracted enormous attention from the researchers in various field of science. However, there exist few examples in the shape control of organic nanostructures. Here in we report on the self-assembled organic nanostructures based on  $\beta/\alpha$ -peptide foldamer, which is a chimeric peptide. The structures and physical properties of the molecular architecture will be presented.



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## Sensing of cyanide using highly selective thiazole-based $\text{Cu}^{2+}$ chemosensor

Aasif Helal, 김현곤, 김홍석

경북대 응용화학과

A new thiazole-based chemosensor (1) was synthesized for the detection of  $\text{CN}^-$  by the displacement of copper from the  $\text{Cu(II)}$  complex of 1. The chemosensor 1 and its copper complex show high selectivity toward  $\text{Cu}^{2+}$  and  $\text{CN}^-$  respectively in aqueous ethanol media. The sensor shows a fluoroionophoric “switch - off” on  $\text{Cu}^{2+}$  and “switch - on” on  $\text{CN}^-$  recognition.

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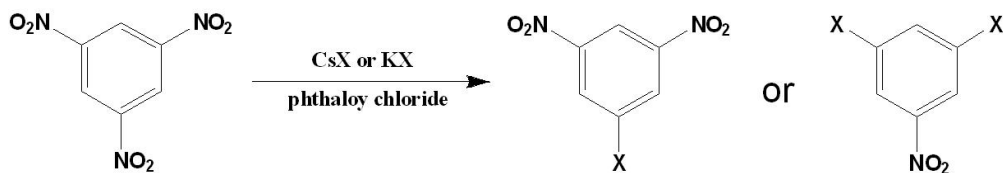
발표종류: 포스터, 발표일시: 목 15:00~17:00

## Synthesis of aromatic halogen compounds from Trinitrobenzene using phthaloyl chloride and X<sup>-</sup>

이웅희, \*함미정, \*Dagvajantsan Oyuner, \*김석찬

국민대 생명나노화학과 \*국민대 화학과

1,3,5-trinitrobenzene 을 출발물질로 사용하고 lithium halide, sodium halide, potassium halide, cesium halide 과 phthaloyl chloride 를 이용하여 halogen contained nitrobenzene 을 합성하였다. 이는 nitro group 을 amine 으로 환원하여 Sandmeyer reaction 을 통한 halogen 의 도입에 비하여 훨씬 간단하며, 높은 수율로 product 를 얻을 수 있다.



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## **TiCl(O<sup>i</sup>Pr)<sub>3</sub> mediated one-pot reductive amination of 1,1'-diacetylferrocene with aryl amine**

**Md. Wasi Ahmad, 김홍석**

경북대 응용화학과

A procedure for one-pot reductive amination of 1,1'-diacetylferrocene with aryl amines in the presence of TiCl(O<sup>i</sup>Pr)<sub>3</sub>-NaBH(OAc)<sub>3</sub> was developed. TiCl(O<sup>i</sup>Pr)<sub>3</sub>-NaBH(OAc)<sub>3</sub> system converted 1,1'-diacetylferrocene with various aryl amines to 1,1'-diarylamioferrocene in good yields of up to 82% at room temperature.

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## **A new acridine-imidazolium based-cholestane receptor for anion sensing**

**Jadav 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. Imidazolium functionalized receptors have recently gained a great deal of attention due to many of their derivatives are capable of binding anions through strong  $(\text{C-H})^+ \cdots \text{X}^-$  interaction. A new fluorescent cholestane-based imidazolium receptor bridged with 1,8-dimethyleneacridine has been synthesized and assessed its binding properties toward anions.

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## Photo-switchable Dyad, Triad, and Pentad Consisting of Porphyrin and Spiropyran Units

박태종, 신은주

순천대 화학과

Spiropyran is well-known photochromic compound accomplishing molecular structural change to merocyanine form by the reversible photochemical cleavage of the C-O bond in the spiropyran ring on UV irradiation. In turn, merocyanine is transformed to spiropyran by ring closure, thermally or on irradiation of visible light. Reversible photochromic spiropyran-merocyanine transformation is one of the subject of active research on optical memory and switch. Because absorption spectra of two isomeric molecules are significantly different, the color change is the most spectacular evidence of photochromism. Besides this color change, many molecular and bulk properties also change in the case of incorporating photochromic molecules into organic materials. Incorporating photochromic molecules into organic materials leads to a variety of photoresponsive systems, the properties of which can be manipulated by light. Porphyrin is one of most frequently employed photoactive molecules due to its spectral and redox properties. A number of artificial light-harvesting antenna, long-range electron transfer systems, and molecular energy storage devices including porphyrins have been investigated. In this study, porphyrin-spiropyran dyad, porphyrin-(spiropyran)<sub>2</sub> triad, and porphyrin-(spiropyran)<sub>4</sub> pentad were prepared and the properties were investigated.

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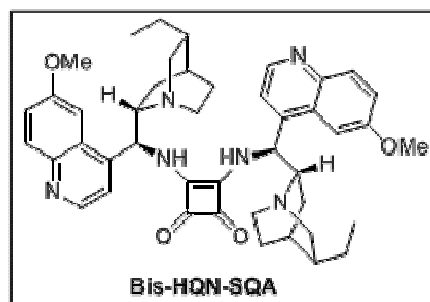
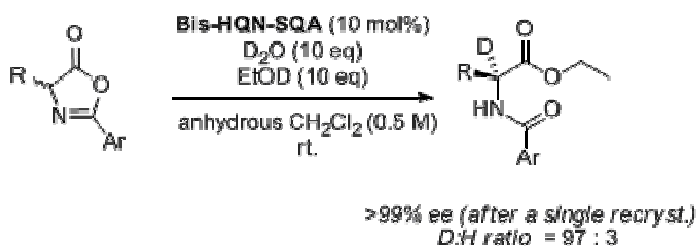
발표종류: 포스터, 발표일시: 목 15:00~17:00

## Enantioselective Synthesis of $\alpha$ -Deuterium Labelled Chiral $\alpha$ -Amino Acids via Dynamic Kinetic Resolution of Racemic Azlactones Catalyzed by Squaramide-Based Dimeric Cinchona Alkaloids

오중석, 송충의

성균관대 화학과

We report an efficient method for the synthesis of  $\alpha$ -deuterium labelled chiral amino acids via dynamic kinetic resolution (DKR) reaction of racemic azlactones using a bifunctional, squaramide-based dimeric cinchona alkaloid organocatalysts. For example, in the presence of a mixture of EtOD/D<sub>2</sub>O, the N-protected  $\alpha$ -deuterated amino esters were obtained 78-90% ee and deuterium to hydrogen ratio was 97-98%. After a single recrystallization, the N-protected- $\alpha$ -deuterated amino esters were obtained in enantiomerically pure form (>99% ee). Moreover, the poor solubility of the catalysts in organic solvents enables their easy recovery after the reaction by a simple precipitation method, allowing their repeated recycling without any loss of turnover number or enantioselectivity.



일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: II-ORGN.P-277

발표분야: 유기화학

발표종류: 포스터, 발표일시: 목 15:00~17:00

## **4,4',4''-Tris(4-naphthalen-1-yl-phenyl)amine as a multifunctional material for organic light-emitting diodes, organic solar cells, and organic thin-film transistors**

권종철, 홍종인

서울대 화학부

We have developed the first multifunctional organic material, 4,4',4''-tris(4-naphthalen-1-yl-phenyl)amine (1-TNPA), which can be used as a deep blue emitting and hole-transporting material in organic light-emitting diodes (OLEDs), as a donor material in organic solar cells (OSCs), and as an active material in organic thin-film transistors (OTFTs). In particular, 1-TNPA-based OLEDs exhibited deep-blue light emission similar to the NTSC standard blue, and more efficient hole transport characteristics than that in the case of NPD-based OLEDs. 1-TNPA can be also used as a donor in OSCs and as an organic semiconductor in OTFTs.

일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: II-ORGN.P-278

발표분야: 유기화학

발표종류: 포스터, 발표일시: 목 15:00~17:00

## **4,4'-Dipyrenyl-biphenyl as an efficient active material for organic light-emitting diodes and organic thin-film transistors**

권종철, 이성훈, 홍종인

서울대 화학부

We have demonstrated an efficient and thermally stable material (4,4'-dipyrenyl-biphenyl, DBP) for both deep blue emitting material in organic light-emitting diodes (OLEDs) and active channel layer in organic thin-film transistors (OTFTs). The 3% DBP doped device showed a blue emission with the Commission Internationale de l'Eclairage (CIE) of (0.15, 0.13) and efficient current efficiency of 3.9 cdA<sup>-1</sup> in OLEDs. Furthermore, the DBP-based OTFTs showed a good field-effect mobility of 0.21 cm<sup>2</sup> V<sup>-1</sup>s<sup>-1</sup>, threshold voltage of -16.9 V, and an on/off current ratio of  $2.0 \times 10^6$  with octadodecyltrichlorosilane-treated SiO<sub>2</sub> layer at 19 °C, respectively.



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장소: 제주ICC

발표코드: II-ORGN.P-279

발표분야: 유기화학

발표종류: 포스터, 발표일시: 목 15:00~17:00

## Functionalized Organic Dyes Comprising 1H-Phenanthro[9,10-d]imidazole Donor for Dye-Sensitized Solar Cells Applications

양유나, \*조나라, \*고재중, 홍종인

서울대 화학부 \*고려대 소재화학과

In recent years, considerable attention has been paid to renewable natural energy sources due to a remarkable increase in worldwide energy consumption. Dye-sensitized solar cells (DSSCs) have received much attention as low cost next-generation solar cells. Compared to ruthenium based dyes, organic dyes have a variety of advantages such as large molar extinction coefficient, easy modification of molecular structures, relatively low material costs and environmentally friendly properties. 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. Herein, we report on five functionalized organic dyes comprising 1H-Phenanthro[9,10-d]imidazole as a electron donor and cyanoacetic acid as a anchoring group which are linked by  $\pi$ -conjugated bridges such as phenylene and thiophenylene moieties, and device data of the DSSCs was fabricated using the five dyes. 1H-Phenanthro[9,10-d]imidazole not only exhibits good electron-donating ability, but also spatially separates the oxidized dye from the TiO<sub>2</sub> surface which efficiently retards charge recombination. By incorporating butylphenyl on the donor moiety, we expected an increase in the electron donating ability which facilitates stronger intramolecular charge transfer (ICT) and a red shift of the absorption region as well as suppressing dye aggregation. Further, we designed a dye containing polyethylene glycol chains which coordinate Li<sup>+</sup> ions and thus minimize charge recombination. In order to realize an wide-range absorption, we combined a squaraine dye with a donor moiety so that the absorption range can be extended up to near-IR region. The effect of the number of phenylene and functionalized moieties on the photophysical, electrochemical properties as well as photovoltaic performance was systematically investigated.

일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: II-ORGN.P-280

발표분야: 유기화학

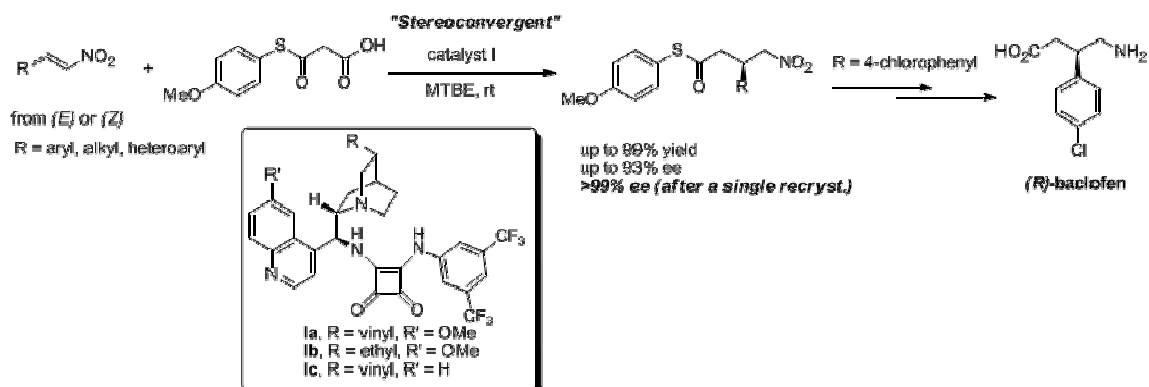
발표종류: 포스터, 발표일시: 목 15:00~17:00

## Biomimetic Organocatalytic Enantioselective Michael Addition of Malonic Acid Half Thioesters to Nitroolefins: An Effective Process for Synthesis of $\gamma$ -Amino Acid Precursors

배한용, \*Surajit Some, \*송충의

성균관대 자연과학부 화학과 \*성균관대 화학과

We will report that cinchona-based squaramides **I** serve as remarkably effective catalysts for the biomimetic enantioselective Michael addition reactions of malonic acid half thioesters (MAHTs) to a variety of nitroolefins, affording optically active  $\gamma$ -amino acid precursors **II** in excellent yields and enantioselectivities. Interestingly, this process is enantioconvergent, a highly desirable feature of a catalytic asymmetric reaction, where a mixture of stereo-isomers affords only one product enantiomer. In addition, the synthetic utility of our protocol was demonstrated in the synthesis of pharmaceutically important  $\gamma$ -amino acids such as (*R*)-baclofen. Details of the mechanistic hypothesis and the basis for enantioselectivity will also be presented.



일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: II-ORGN.P-281

발표분야: 유기화학

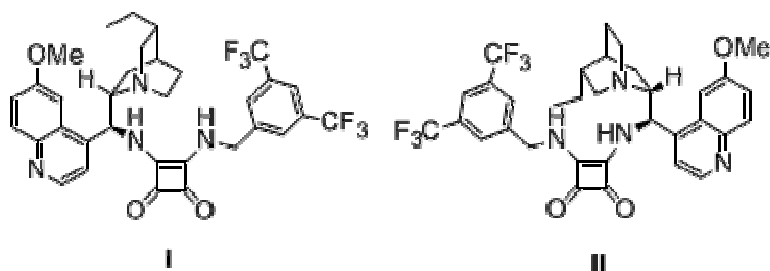
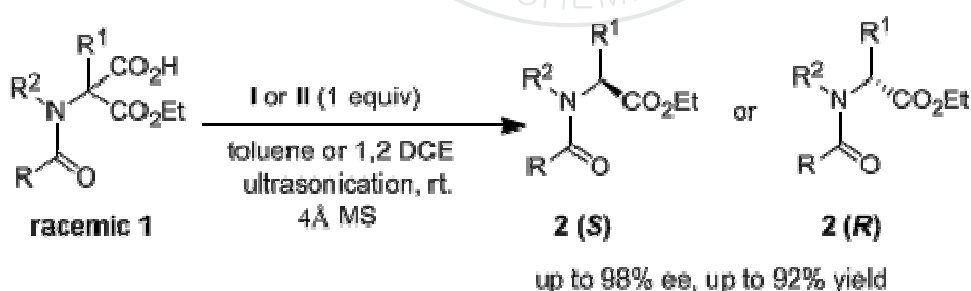
발표종류: 포스터, 발표일시: 목 15:00~17:00

## Asymmetric Synthesis of $\alpha$ -Amino Esters via Cinchona-Mediated Enantioselective Decarboxylative Protonation of Racemic $\alpha$ -Aminomalonic Acid Half Esters

Surajit Some, 송충의

성균관대 화학과

Unprecedentedly high enantioselectivities (up to 98% ee) for the enantioselective decarboxylative protonations of racemic  $\alpha$ -aminomalonic acid half esters **1** has been obtained by employing squaramide-based cinchona alkaloids, I and II. Optimization of the reaction conditions revealed that the reaction time can be dramatically reduced under sonication conditions. Moreover, the use of molecular sieves showed the positive effect on enantioselectivity. We have used our method to obtain optically enriched cyclic and acyclic amino acid derivatives **2** that are not readily prepared by other bio- and chemocatalytic methods.



일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: II-ORGN.P-282

발표분야: 유기화학

발표종류: 포스터, 발표일시: 목 15:00~17:00

## Synthesis of Poly(lactic acid) Copolymer

김성호, \*이혁, \*\*민보라, \*\*\*임정연

한국화학연구원 신물질연구본부 의약화학연구센터 \*한국화학연구원 신약연구단 \*\*성균관대  
화학과 \*\*\*한국화학연구원 화학과

In recent years, there has been a great need for biodegradable polymeric materials, since waste polymers cause destruction of the environment. Poly(lactic acid) is the most widely studied biodegradable polymer. However, its lower thermal and mechanical properties provide obstacles to its wide applications. For this reason, Many researcher have been reported various poly(lactic acid) copolymers to improve it. We incorporated aromatic moiety into poly(lactic acid) skeleton via synthesizing novel monomers composed of lactic acid and phenylacetic acid. The ratio of lactic acid and aromatic group in monomers could be controlled by the manipulation of deprotection steps. Also, we could control the chirality of monomer by same synthetic strategy. The polymerization of those monomers affords diverse poly(lactic acid) copolymers.

일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: II-ORGN.P-283

발표분야: 유기화학

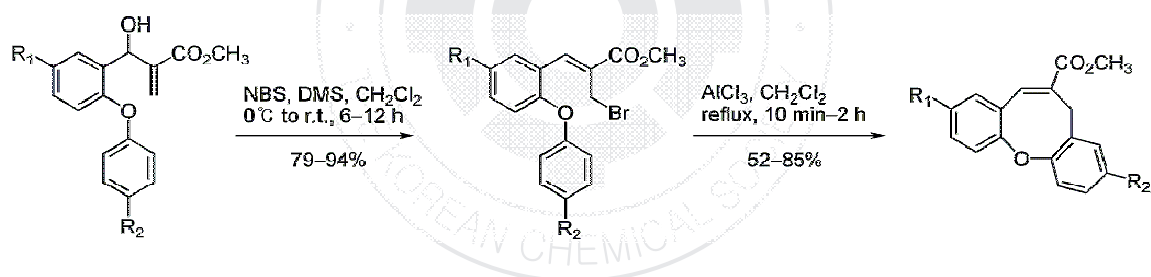
발표종류: 포스터, 발표일시: 목 15:00~17:00

## Baylis–Hillman Route to Methyl 7*H*-Dibenz[*b,g*]oxocin-6-carboxylates

안상현, 장승순, 이기정

한양대 화학공학과

A simple method for synthesizing several methyl 7*H*-dibenz[*b,g*]oxocin-6-carboxylates via Friedel–Crafts reaction of readily available bromides of Baylis–Hillman adducts with aluminum chloride has been described.



일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: II-ORGN.P-284

발표분야: 유기화학

발표종류: 포스터, 발표일시: 목 15:00~17:00

## **A Practical Metal-Free Approach for the Amination of Azoles through an Unprecedented Ring-Opening and Closing Strategy**

**Jomy Kuruthukulangar**, 김지영, 장석복

KAIST 화학과

A new metal-free protocol for the amination of azoles has been developed using iodobenzenediacetate to couple various types of azoles with amines (see scheme). The reaction proceeds via ring-opening and subsequent closing pathway in the absence of metallic reagents and acid or base additives. Optimal reaction conditions are very mild, and substrate scope is broad, thus producing a wide range of 2-aminoazoles, an important pharmacophore of high bioactivities, in high efficiency.



일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: II-ORGN.P-285

발표분야: 유기화학

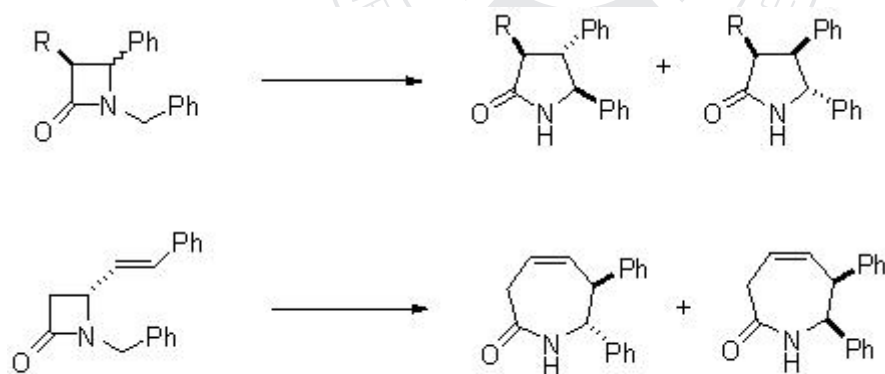
발표종류: 포스터, 발표일시: 목 15:00~17:00

## Stereoselective Syntheses of various Lactam Derivatives via Ring Expansion of $\beta$ -Lactam Derivatives.

김미형, 장석명, 안철진

창원대 화학과

The  $\gamma$ -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  $\epsilon$ -lactam derivatives with vinyl substituents on C-4 has been investigated too.





일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: II-ORGN.P-286

발표분야: 유기화학

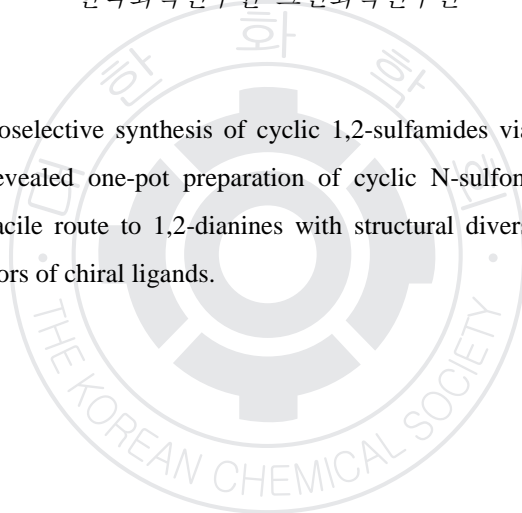
발표종류: 포스터, 발표일시: 목 15:00~17:00

## **A facile route to chiral 1,2-diamines via Rh-catalyzed transfer hydrogenation of cyclic N-sulfonylimines**

이선아, 이기인

한국화학연구원 그린화학연구단

We achieved highly enantioselective synthesis of cyclic 1,2-sulfamides via rhodium-catalyzed transfer hydrogenation, and also revealed one-pot preparation of cyclic N-sulfonylimines from  $\alpha$ -hydroxy ketones. This afforded a facile route to 1,2-dianines with structural diversity, which are useful chiral building blocks and precursors of chiral ligands.





일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: II-ORGN.P-287

발표분야: 유기화학

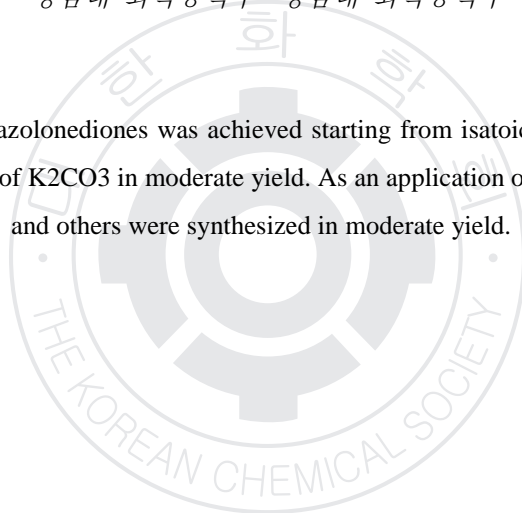
발표종류: 포스터, 발표일시: 목 15:00~17:00

## One-Step Synthesis of Quinazolonediones: First Synthesis of Goshuyuamide II

LI XIN, \*이용록

영남대 화학공학부 \*영남대 화학공학부

One-Step synthesis of quinazolonediones was achieved starting from isatoic anhydride with amines and triphosgene in the presence of K<sub>2</sub>CO<sub>3</sub> in moderate yield. As an application of this methodology, naturally occurring Goshuyuamide II and others were synthesized in moderate yield.



일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: II-ORGN.P-288

발표분야: 유기화학

발표종류: 포스터, 발표일시: 목 15:00~17:00

## Correlation of the Specific Rates of Solvolysis of 1-Adamantylmethyl Chloroformate Using the Grunwald-Winstein Equation

이예린, 문두환, \*유찬주, \*\*경진범

한양대 응용화학과 \*한양대 \*\*한양대 과학기술대학 응용화학과

The specific rates of solvolysis of 1-adamantylmethyl chloroformate(1-AdCH<sub>2</sub>OCOC<sub>2</sub>H<sub>5</sub>, **1**) are reported at 40.0°C in a variety of pure and binary aqueous organic mixtures with wide ranging nucleophilicity and ionizing power values. For **1**, we also report the specific rates determined at different temperatures for pure ethanol (EtOH), methanol (MeOH), 80% EtOH, and 70% 2,2,2-trifluoroethanol (TFE), and the solvent deuterium isotope effect,  $k_{\text{MeOH}}/k_{\text{MeOD}}$  at 40.0°C in methanol. The enthalpy ( $\Delta H^\ddagger$ ) and entropy ( $\Delta S^\ddagger$ ) of activation values obtained from Arrhenius plots for **1** in these four solvents are reported. The specific rates of solvolysis of **1** are analyzed using the extended Grunwald-Winstein equation ( $\log(k/k_0) = \rho \ln + mY + c$ ), and estimated the relative contributions to the overall reaction from ionization pathway and addition-elimination pathway. The results are also compared with those previously reported for the corresponding primary, secondary, and tertiary alkyl chloroformate esters.

일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: II-ORGN.P-289

발표분야: 유기화학

발표종류: 포스터, 발표일시: 목 15:00~17:00

## Rate and Product Studies of 1-Adamantyl Fluorothioformate Under Solvolytic Conditions

성미혜, 이용우, \*경진범

한양대 응용화학과 \*한양대 과학기술대학 응용화학과

Alkyl haloformate and halothioformate esters are important reagents which are widely used in physiological and biological studies. A recently study of 1-adamantyl chlorothioformate (1-AdSCoCl, **1**) is extended to 1-adamantyl fluorothioformate (1-AdSCoF, **2**). The specific rates of solvolysis of **2** in hydroxylic solvents have been studied by autotitrimetric method. The simple and extended Grunwald-Winstein equations have been applied to the specific rates of solvolysis of **2** over the full range of solvents. For five solvents, studies were made at several temperatures and activation parameters determined. The results are compared with those reported earlier for 1-adamantyl chloroformate (1-AdOCOC1), 1-adamantyl fluoroformate (1-AdOCOF), and alkyl chlorothioformate esters.

일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: II-ORGN.P-290

발표분야: 유기화학

발표종류: 포스터, 발표일시: 목 15:00~17:00

## Fluorescent Chemosensor discriminating phosphate-containing biomolecules by PeT mechanism

오진록, 홍종인

서울대 화학부

Phosphate-containing biomolecules are recognized as important molecules in a living system because of their roles involved in signal transduction, energy currency and control of metabolic processes and so on. Also, many of these processes are usually conducted with a concomitant release of pyrophosphate by the enzymatic reactions of NTPs using kinases. For this reason, it is important to develop a fluorescent chemosensor that can distinguish pyrophosphate from NTPs. It has been known that the intrinsic fluorescence of the isoalloxazine unit is intramolecularly quenched by a nearby quenching unit, as revealed in the case of FAD. FAD is nonfluorescent in aqueous solution by the PeT (Photoinduced-electron-Transfer) from the adenine base to isoalloxazine. Here, we report a new fluorescent chemosensor bearing 2,2'-dipicolylamine-Zn(II) complex and an isoalloxazine ring system that can discriminate phosphate-containing biomolecules.

일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: II-ORGN.P-291

발표분야: 유기화학

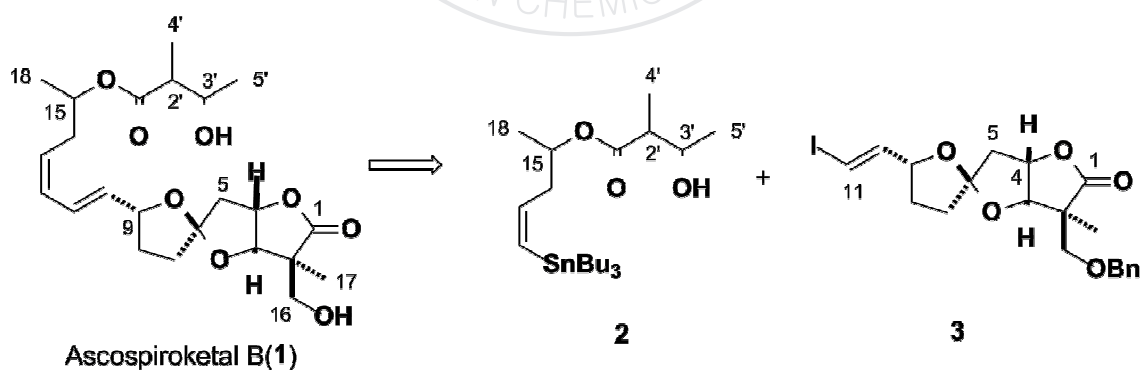
발표종류: 포스터, 발표일시: 목 15:00~17:00

## Studies Toward the Total Synthesis of Ascospiroketal B

김종우, 이정열, 한서정, 이덕형

서강대 화학과

Ascospiroketal B(1) was isolated from the marine-derived fungus *Ascochyta salicorniae*, which was cultivated under OSMAC approach by Gabriele M. König et. al in 2007. Ascospiroketal B possesses a rare tricyclic core skeleton with a quaternary carbon at C2 and chiral spiroketal at C6, and a total of 8 stereogenic centers. A key intermediate containing  $\gamma$ -butyrolactone was found to be unstable from our studies. We report herein a new synthetic study in which  $\gamma$ -butyrolactone was introduced at a later stage. Our synthetic strategy for ascospiroketal B(1) involves the assemble of vinyl stanne 2 and vinyl iodide 3 by Stille coupling. Synthetic route to vinyl iodide 3 involves asymmetric alkylation using chiral auxiliary as a key step, ketalization under acidic condition, and lactonization for construction of  $\gamma$ -butyrolactone.



일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: II-ORGN.P-292

발표분야: 유기화학

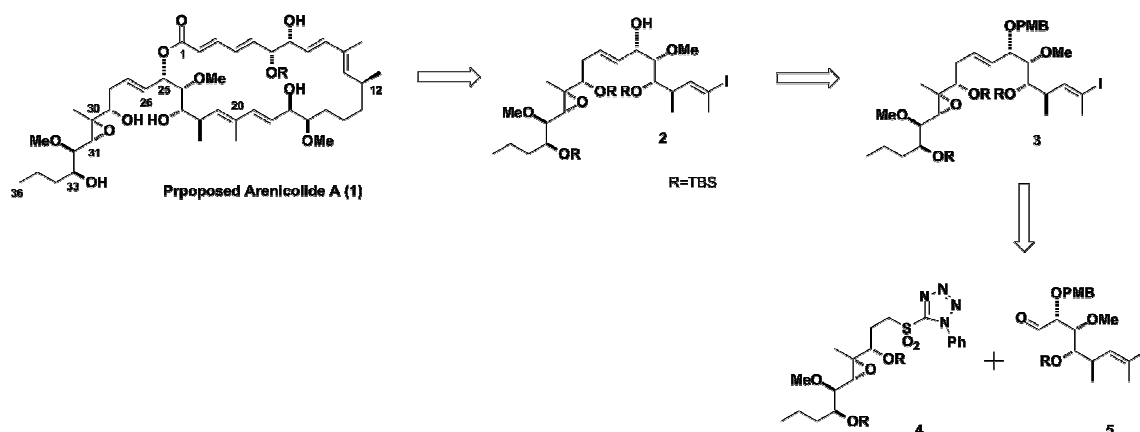
발표종류: 포스터, 발표일시: 목 15:00~17:00

## A challenge for the Total Synthesis of Arenicolide A

이정열, 이광국, 이덕형

서강대 화학과

Arenicolide A, a 26-membered macrolide with anti-cancer activity, was isolated from the large-scale fermentation of the *S. arenicola* in 2007. Recently, the synthesis of fragment 4 and 5 were completed. And then we focused on the coupling between sulfone 4 and aldehyde 5 by Julia-Kocienski olefination. However, the Julia coupling raised an unexpected challenge. Traditional (*E*)-selective condition(KHMDS/DME) furnished (*E*)-alkene 2 with low diastereoselectivity(1:1), albeit in excellent yield. The (*E/Z*) selectivity was improved by somewhat addition of 18-crown-6 the traditional reaction condition(2:1).(*E*)-alkene 2 was produced by deprotection of PMB group with DDQ, the corresponding  $\alpha,\beta$ -unsaturated ketone was also isolated by excess DDQ. Fortunately, Chelation-controlled reduction of the ketone with  $\text{Zn}(\text{BH}_4)_2$  gave the desired alcohol 2. New synthetic route from these studies will be presented in due course





일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: II-ORGN.P-293

발표분야: 유기화학

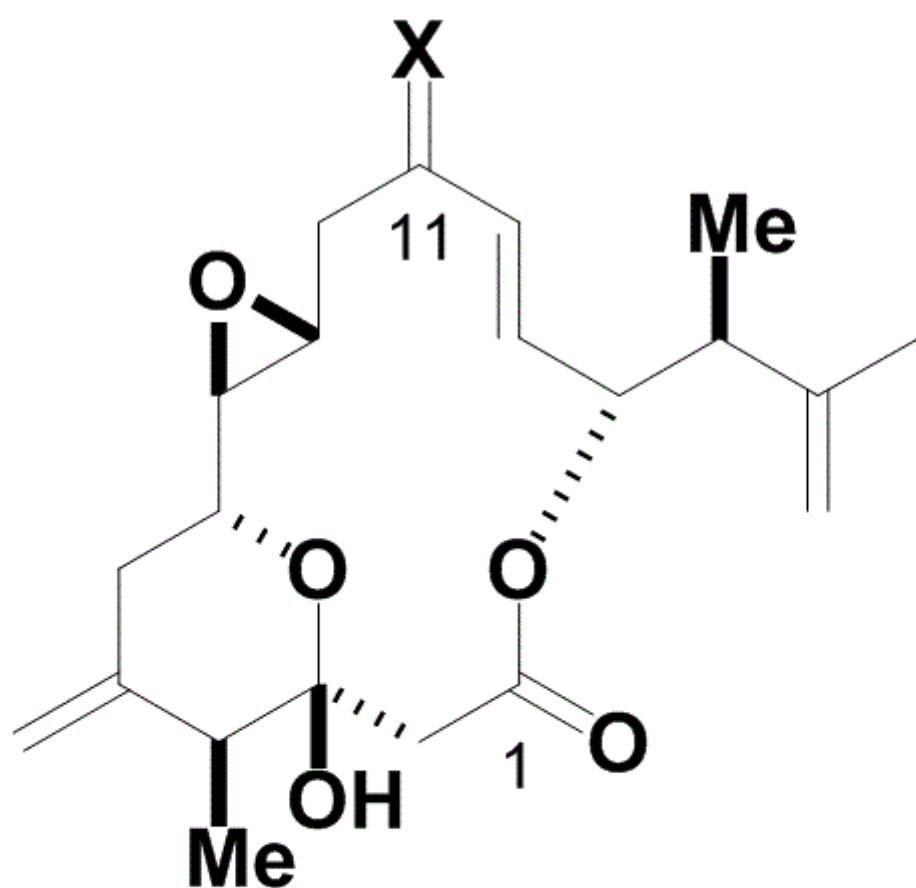
발표종류: 포스터, 발표일시: 목 15:00~17:00

## Convergent Approaches towards the Total Synthesis of Amphidinolide O and P

황민호, 한서정, \*하나름, 이덕형

서강대 화학과 \*건양대 나노바이오화학과

A diflagellate *Amphidinolium* sp. from Okinawan marine contains many macrolides named amphidinolides. These macrolides is particularly attracted from synthetic community because of their cytotoxic activities against various cancer cell lines. Amphidinolide P is a 15-membered macrolide possessing 7-chiral centers, one epoxide, one internal double-bond, and two exo-methylene (C5, C11) in the macro-lactone ring. Amphidinolide O has ketone on the C11. We planned convergent strategy for complete of amphidinolide O and P in the same route. Amphidinolide O could be completed by the sequential synthesis of two exo-methylene of amphidinolide P in the latter part.



**X = O : amphidinolide O (1)**  
**X = CH<sub>2</sub> : amphidinolide P (2)**

일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: II-ORGN.P-294

발표분야: 유기화학

발표종류: 포스터, 발표일시: 목 15:00~17:00

## **Application of controlled cyclization with sulfone group to the natural compound.**

서정아, \*구상호

명지대 나노공학과 \*명지대 화학과

Most all of the medicinally and biologically important compounds in nature have a ring structure, mono-cyclic, bi-cyclic, poly-cyclic etc. Construction of ring structures is important in organic synthesis. We were interested in controlling the mode of cyclization. We have studied a chain-extension method mediated by a sulfone group. I was envisioned that the internal sulfone group would efficiently control the mode of cyclization by interfering the chain molecule with folding. We efficiently synthesized mono-cyclic natural compound containing a long isoprenoid chain by the controlled cyclization with sulfone group.

일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: II-ORGN.P-295

발표분야: 유기화학

발표종류: 포스터, 발표일시: 목 15:00~17:00

## Construction of Allylic sulfone containing phenyl substituents for the Unnatural carotenoids.

임보람, 오은택, \*구상호

명지대 나노공학과 \*명지대 화학과

The stability and electronic characteristics of the conjugated polyene chains containing aromatic substituents were compared with those of the natural carotenoids. aromatic end-groups and aromatic substituents were attached to the conjugated polyene chain, thereby utilizing the stabilized carotenoid compounds as excellent materials for conductive organic molecules, organo-electric circuit. Allylic sulfone unit is used as a useful material in the synthesis of diversely substituted carotenoid compound. For the construction of allylic sulfone, we should construct allylic chloride unit containing various substituent. The homoallylic alcohol containing homoallylic sulfone moiety can be prepared by the Indium-mediated addition of Allylic chloride unit to aldehyde. The reaction provides high stereoselectivity as well as an absolute regioselectivity. This homoallylic alcohol produces the allylic sulfone containing the conjugated polyenes by the Oxonia-Cope rearrangement using new Lewis acid. This method using new Lewis acid is overcome several weak point that is prins product. Also It progress in a way that is more mild condition.

일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: II-ORGN.P-296

발표분야: 유기화학

발표종류: 포스터, 발표일시: 목 15:00~17:00

## Control of regioselectivity in the esterification of glycerol

최보슬, \*구상호

명지대 나노공학과 \*명지대 화학과

Phosphatidylcholine is one of the main component of biological membranes. A typical phosphatidylcholine has hydrophobic tail consisted of two fatty acyl chains esterified to two adjacent hydroxyl groups in glycerol and a polar head group, phosphate group and choline attached to the other hydroxy group. Since glycerol consists of three hydroxyl groups, it is not easy to synthesize diglycerides regioselectively. So, we tried regioselective epoxide ring opening by acid nucleophiles. We were able to synthesize various diglyceride, which would be efficiently utilized for the formation of phosphatidylcholine derivatives.

일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: II-ORGN.P-297

발표분야: 유기화학

발표종류: 포스터, 발표일시: 목 15:00~17:00

## **An Efficient Method of Selective Deoxygenation of Allylic Alcohols**

**Liang Su**, 구상호

명지대 화학과

It is so common that more than one hydroxyl groups existed in one compound. To selectively activate different hydroxyl groups has been a tough job in the organic synthesis field. We have developed a selective method for deoxygenating of the allelic hydroxyl group in the presence of non-activated normal hydroxyl group. Selective reduction method of allelic alcohols proceeds by the formation of 1-alkoxyallyl ethers and Pd-catalyzed, Super Hydride reduction sequence. This selective reduction method has been applied to the synthesis of Lavandulol, which is an important additive in the perfume industry. More details will be discussed during the presentation.

일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: II-ORGN.P-298

발표분야: 유기화학

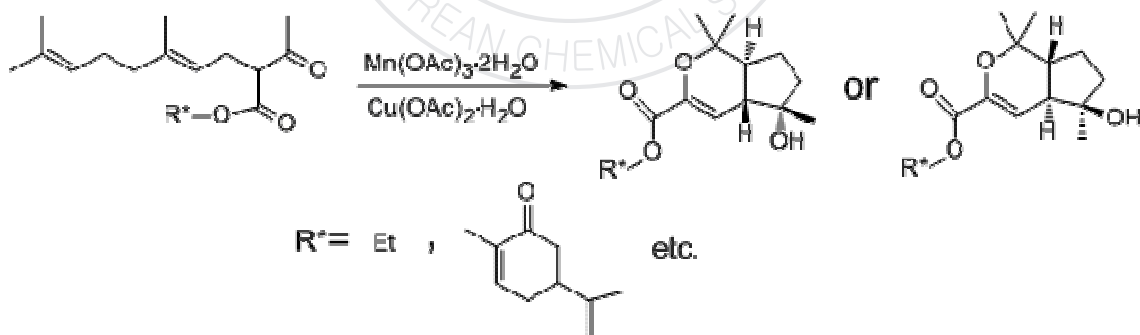
발표종류: 포스터, 발표일시: 목 15:00~17:00

## Mn(III)-initiated enantioselective synthesis of heterocyclic compounds and furan formation

Wang Chao, \*구상호

명지대 나노공학과 \*명지대 화학과

We have devised heterocyclic compounds which could be synthesized from isoprenoid chains via intermolecular Hetero-Diels-Alder reactions that are induced by  $\text{Mn}(\text{OAc})_3 \cdot 2\text{H}_2\text{O}$  and  $\text{Cu}(\text{OAc})_2 \cdot \text{H}_2\text{O}$ . There is high selectivity in this reaction, whereas no enantioselectivity exists. Therefore, the chiral auxiliary groups are attached to the isoprenoid chains so as to make the cyclization enantioselective. In addition,  $\text{Mn}(\text{OAc})_3 \cdot 2\text{H}_2\text{O}$  and  $\text{Cu}(\text{OAc})_2 \cdot \text{H}_2\text{O}$  are developed to form various kinds of furan containing diverse functional groups that may contribute to the synthesis of furan.



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장소: 제주ICC

발표코드: II-ORGN.P-299

발표분야: 유기화학

발표종류: 포스터, 발표일시: 목 15:00~17:00

## **An Efficient Synthetic Route for the Preparation of various carotenoids as the nano wires**

김형준, 전선화, \*구상호

명지대 나노공학과 \*명지대 화학과

The carotenoids are an important class of organic molecules with delocalized  $\pi$ -electrons. A typical carotene molecular wire consists of a polyene backbone of alternating single-double bonds terminated by phenyl rings at the end. We have successfully demonstrated the efficient syntheses of natural carotenoids, and based upon that, we could synthesize unnatural carotenoid wires efficiently. The conjugated polyene chains of the unnatural carotenoids containing aromatic substituents would provide an extra stability and excellent electronic characteristics compared with those of the natural carotenoids. Therefore, we were able to measure electrical conductivity using unnatural carotenoid wires.



일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: II-ORGN.P-300

발표분야: 유기화학

발표종류: 포스터, 발표일시: 목 15:00~17:00

## Hydrogelators Showing Visual Discrimination of Biothiols

장동학

서울대 화학부

For decades, various biothiol sensors/probes have been developed using various mechanisms. However, a few sensors are known that can discriminate between homocystein and cystein. Low molecular-weight gelators (LMWGs) are known to generate various self-assembled superstructures according to their structures, environment, and/or additives. In particular, even a small change in the molecular structure of LMWGs would induce massive changes in self-assembled superstructures. Cystein and homocystein easily form 5- and 6-membered thiazole ring compounds, respectively, by the reaction with coumarin based hydrogelator which has a formyl group (*formyl-C*). The resulting 5- and 6-membered thiazole ring compounds showed different gelation behavior, which in turn resulted in successful discrimination between homocystein and cystein. This study clearly revealed that a small structural difference in the reaction products between biothiol and *formyl-C* induced massive changes in the self-assembled process.

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장소: 제주ICC

발표코드: II-ORGN.P-301

발표분야: 유기화학

발표종류: 포스터, 발표일시: 목 15:00~17:00

## Colorimetric and Fluorometric Sensor for Surfactants Based on Conjugated Polydiacetylenes

전혜령, \*윤주영

이화여대 화학나노과학 \*이화여대 화학과

Polydiacetylene(PDA) is a colorimetric polymer owing to a brilliant blue-to-red color transition that takes place in response to environmental perturbations. Also, it already has been known that “blue-phase” PDAs are nonfluorescent while their “red-phase” counterparts fluorescence. Owing to the color (blue-to-red) and fluorescence (non-to-fluorescent) changes, PDAs have been actively used as sensory materials for the detection of biologically, environmentally, and chemically-important target molecules. Diacetylene amphiphiles are self-assembled into a variety of forms that can be modified for various detection applications, and be photopolymerized to generate PDA in situ. PDA provides optical signal generation arising from changes in the absorption and emission spectra of the conjugated backbone caused by interaction with the target materials. In this current presentation, we prepared a series of new PDAs which bear either benzoic acid head groups or amine moieties as head groups. They show different colorimetric changes upon the different lengths and head groups of surfactants. We demonstrated our system is a simple and selective method to detect surfactant in water.

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장소: 제주ICC

발표코드: II-ORGN.P-302

발표분야: 유기화학

발표종류: 포스터, 발표일시: 목 15:00~17:00

## Bi-Nuclear Boron Complexes Based on Pyrene Ligand: Strong Solid/Liquid Fluorescence and Deep LUMO Level

정지영, \*김동하, \*\*이종목, \*\*윤주영

이화여대 바이오융합과학과 \*이화여대 화학나노과학과 \*\*이화여대 화학과

Organic fluorine-boron complexes, BODIPY (dipyrro-boradiazaindacenes) being the best-known example, have intense fluorescence and tunable emission wavelengths. However, BODIPY and its derivatives have severe limits to applications to organic light-emitting diodes (OLED). Boron complexes with high solid state emission intensity showed potential as an electron transporting material in OLEDs or dye-sensitized solar cells. Therefore, there is a need to develop novel boron complexes with a well-designed structure to overcome the weakness of BODIPY and control the optical properties, improve their electron-accepting capability and apply them successfully to OLEDs. Bi-nuclear boron complex centers not only insure strong fluorescence intensity but also form a strong electron-acceptor moiety with a deep LUMO level to facilitate electron-transport. Novel bi-nuclear boron complexes 1-3 with a pyrene ligand have significant features, such as strong fluorescence in solution and solid state, lower LUMO and higher HOMO levels. And thin films of compound 2 were confirmed by atomic force microscopy (AFM) to be continuous and well-formed, making this compound suitable for the further OLED studies. These novel boron complexes are multifunctional candidates for use in light-emitting or electron transporting applications.

일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: II-ORGN.P-303

발표분야: 유기화학

발표종류: 포스터, 발표일시: 목 15:00~17:00

## Novel Imidazolium-Containing Fluorescent Chemosensor for the Recognition of Anions

최지영, \*윤주영

이화여대 바이오융합과학(화학) \*이화여대 화학과

Anions play a crucial role in a wide range of chemical and biological processes, and considerable effort has been devoted to the development of abiotic receptors for anionic species. The imidazolium group has been actively studied for the recognition of anions. The imidazolium receptors bind anions by forming C-H...X- hydrogen bonds, wherein the charge-charge electrostatic interaction dominates, and thus this type of charged hydrogen bonding is very intriguing in comparison with many other types. In the design of the target molecules, the imidazolium receptors were linked to fluorophores. The novel imidazolium containing derivatives showed fluorescent change when bound with anions such as fluoride, acetate, and dihydrogen phosphate. Thus these molecules are expected to be used as chemosensors which sense important anions.

일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: II-ORGN.P-304

발표분야: 유기화학

발표종류: 포스터, 발표일시: 목 15:00~17:00

## A Dual Colorimetric and Fluorometric Sensor for Lead Ion Based on Conjugated Polydiacetylenes

이송이, \*Wang Fang, \*\*윤주영

이화여대 바이오융합과학과 \*이화여대 화학.나노과학부 \*\*이화여대 화학과

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. Among the metal ions,  $Pb^{2+}$  is one of the important targets because of the adverse health effects of lead exposure, particularly in children. Since the current lead detection methods, such as atomic absorption spectrometry, inductively coupled plasma mass spectrometry, and others are costly and time demanding processes, a simple method for detecting lead is needed. Compared to lead selective fluorescent sensors, there are only a few examples of lead selective colorimetric sensors and even fewer examples of colorimetric sensors which work in aqueous solution are available. Certainly, naked-eye detection is the simplest process that can be applied for environmental purposes. We report the first example of a  $Pb^{2+}$  selective PDA sensor. In 100% aqueous solution, the presence of lead can be easily monitored via naked-eye detection. In addition, a fluorescence enhancement was observed upon the addition of lead ions.

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발표코드: II-ORGN.P-305

발표분야: 유기화학

발표종류: 포스터, 발표일시: 목 15:00~17:00

## Colorimetric Detection of Copper(II) Based on Polydiacetylene in Water

xu qingling, \*윤주영

이화여대 화학나노과학과 \*이화여대 화학과

A new polydiacetylene(PDA) lipid containing terminal copper-selective groups has been prepared. Cu(I) obtained from reduction of Cu(II) can catalyze the conjugation of the functional groups. The color of PDA solution changed from blue to red after incubation with  $\text{Cu}^{2+}$  and ascorbic acid under room temperature for 1 day, while there was slight color change when incubated with other metal ions. The color change is attributed to conformational transition of conjugated backbone. This provides a new method for naked eye detection of  $\text{Cu}^{2+}$  in water with high sensitivity.

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장소: 제주ICC

발표코드: II-ORGN.P-306

발표분야: 유기화학

발표종류: 포스터, 발표일시: 목 15:00~17:00

## Ratiometric Fluorescent Chemosensor for Silver Ion at Physiological pH

Wang Fang, \*윤주영

이화여대 화학·나노과학부 \*이화여대 화학과

Bis-pyrene derivative 1, bearing two pyrene and pyridine groups, was synthesized as a ratiometric fluorescent chemosensor for  $\text{Ag}^+$  in aqueous solution. Fluorescent chemosensor 1 displayed a selective ratiometric change with  $\text{Ag}^+$ , which was attributed to the excimer-monomer emissions of pyrenes. A mechanism for the binding mode was proposed based on fluorescent changes, NMR experiments and theoretical calculations.

일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: II-ORGN.P-307

발표분야: 유기화학

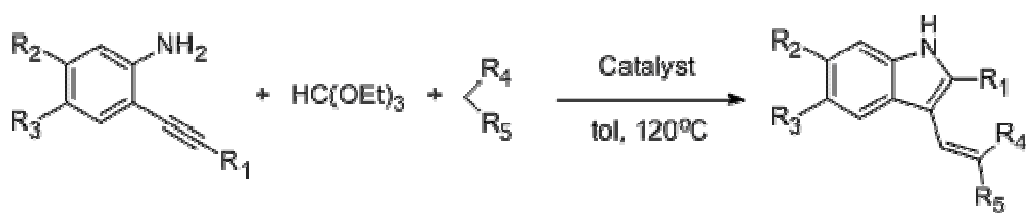
발표종류: 포스터, 발표일시: 목 15:00~17:00

## Synthesis of Various 2,3-disubstituted Indole Derivatives and Its Biological Activities

박효승, 정지선, 김지희, 오창호

한양대 화학과

Substituted indoles are core skeletons in naturally occurring alkaloids and derivatives could widely be used in pharmaceutical field. To date, numerous elegant approaches via transition-metal catalysis have been devoted to generate such unique indole systems. However, only a few syntheses to indole derivatives have been successful by employing intra- or intermolecular cyclization of alkynes and imines. In this presentation, we have developed an efficient domino process for the synthesis of 2,3-disubstituted indoles employing various transition-metal catalyzed three-component cycloisomerization involving 1,3-migration to copper-activated carbon starting from 2-alkynylaniline. And These indole have anti-proliferative activity on human MDA-MB 231 breast cancer cells in a microplate assay.





일시: 2011년 4월 28~29일(목~금) 2일간

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발표코드: II-ORGN.P-308

발표분야: 유기화학

발표종류: 포스터, 발표일시: 목 15:00~17:00

## Highly Controllable 3-Dimensional Molecular Architectures using Self-assembly of $\alpha/\beta$ -Peptide Foldamer

엄재훈, 김양우, 이희승

KAIST 화학과

The self-assembly of peptide-based building blocks into nanostructures is an attractive method for fabricating novel bio-inspired materials because of their capacity for molecular recognition and functional flexibility as well as the mild conditions required in the fabrication process. Various types of self-assembled nano-microstructures by natural or synthetic building blocks are reviewed during the past several years. However, the morphologies of the peptide-based self-assembled nano-microstructures are limited to simple shapes such as spheres, tubes, and rods. In this presentation, we report highly homogeneous and controllable three-dimensional architectures using self-assembly of 1:1-alternating  $\alpha/\beta$ -Peptide foldamer. The controlled morphologies and physical properties will be presented.

일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: II-ORGN.P-309

발표분야: 유기화학

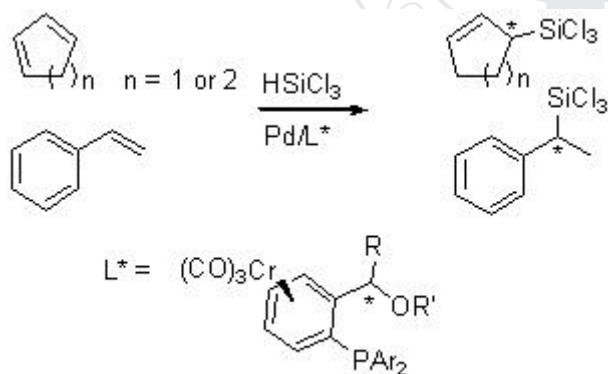
발표종류: 포스터, 발표일시: 목 15:00~17:00

## Pd-catalyzed asymmetric hydrosilylation of styrene and cyclic 1,3-dienes with planar chiral ( $\eta^6$ -arene)chromium monophosphine ligands

신아름, 백희열, 한진욱

한양대 화학과

Palladium-catalyzed asymmetric hydrosilylation of olefins provides one of the most efficient routes to optically active allylsilanes, which are able to be further derivatized to useful synthetic intermediates such as chiral alcohols. Planar chiral ( $\eta^6$ -arene)chromium monophosphine ligands were applied to palladium-catalyzed asymmetric hydrosilylation of styrene and cyclic 1,3-dienes in the study. Enantioselectivities were varied dramatically according to the chiral ligands used.



일시: 2011년 4월 28~29일(목~금) 2일간

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발표코드: II-ORGN.P-310

발표분야: 유기화학

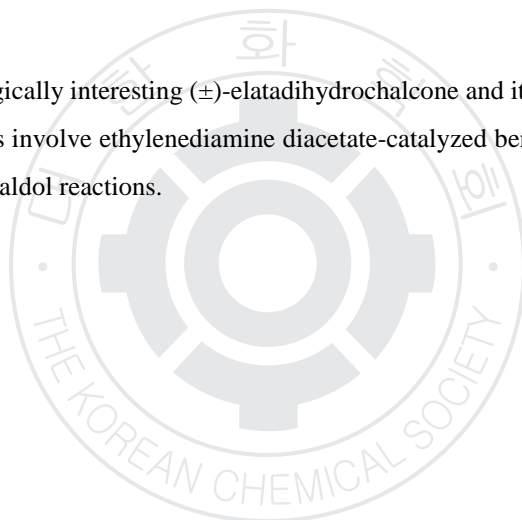
발표종류: 포스터, 발표일시: 목 15:00~17:00

## First Total Synthesis of ( $\pm$ )-Elatadihydrochalcone and Its Analogues

SOMAI MAGAR KRISHNA, 이용록

영남대 화학공학부

The total synthesis of biologically interesting ( $\pm$ )-elatadihydrochalcone and its analogues was successfully achieved. The key strategies involve ethylenediamine diacetate-catalyzed benzopyran formation reactions followed by base-catalyzed aldol reactions.



일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: II-ORGN.P-311

발표분야: 유기화학

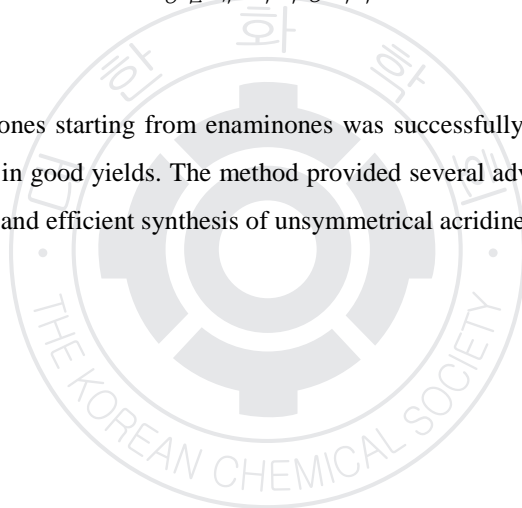
발표종류: 포스터, 발표일시: 목 15:00~17:00

## Efficient Synthesis of Acridinediones by Indium Triflate-Catalyzed Reaction of Enaminones

TO QUANG HUY, 이용록

영남대 화학공학부

The synthesis of acridinediones starting from enaminones was successfully achieved in the presence of indium triflate as a catalyst in good yields. The method provided several advantages such as low catalyst loading, short reaction time and efficient synthesis of unsymmetrical acridinediones.



일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: II-ORGN.P-312

발표분야: 유기화학

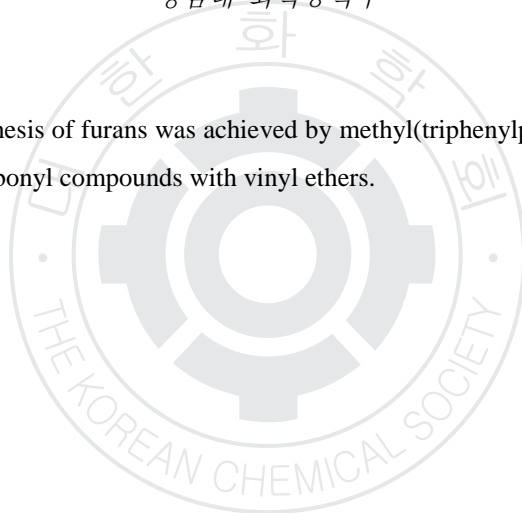
발표종류: 포스터, 발표일시: 목 15:00~17:00

## Efficient Synthesis of Furans by Gold(I)-Catalyzed Cycloaddition of Diazodicarbonyl Compounds

NEUPANE PRATIK, 이용록

영남대 화학공학부

A simple and efficient synthesis of furans was achieved by methyl(triphenylphosphine)gold(I) - catalyzed cycloaddition of diazodicarbonyl compounds with vinyl ethers.



일시: 2011년 4월 28~29일(목~금) 2일간

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발표분야: 유기화학

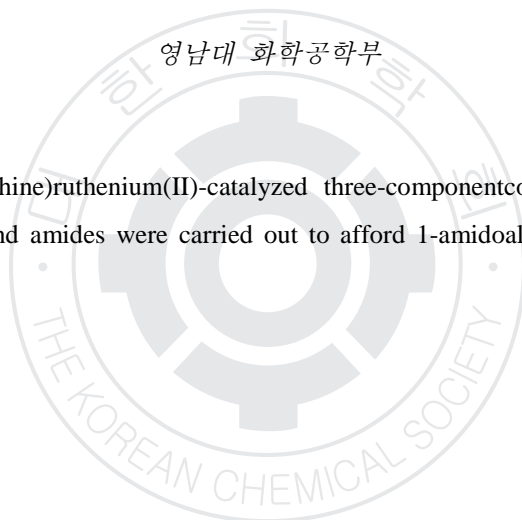
발표종류: 포스터, 발표일시: 목 15:00~17:00

## Synthesis of 1-Amidoalkyl-2-naphthols by Dichlorotris(triphenylphosphine)ruthenium(II) Catalyzed Reaction of 2-Naphthols

주소연, 이용록

영남대 화학공학부

Dichlorotris(triphenylphosphine)ruthenium(II)-catalyzed three-component condensations of 2-naphthols with aromatic aldehydes and amides were carried out to afford 1-amidoalkyl-2-naphthols in moderate yields.



일시: 2011년 4월 28~29일(목~금) 2일간

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발표코드: II-ORGN.P-314

발표분야: 유기화학

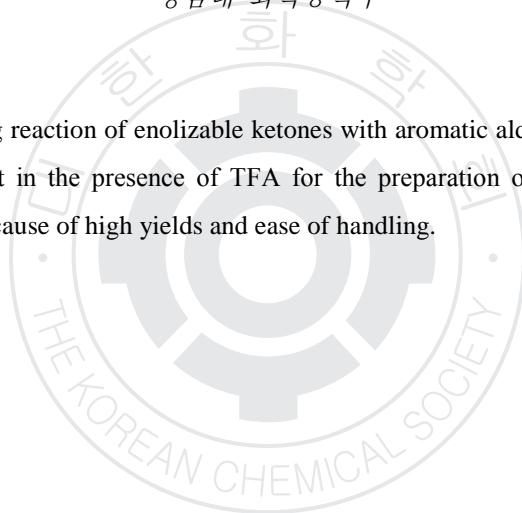
발표종류: 포스터, 발표일시: 목 15:00~17:00

## **TFA-Mediated Multicomponent Condensation for the Synthesis of $\beta$ -Acetamido ketones**

**PANDIT RAMESHWAR PRA, 이용록**

영남대 화학공학부

A multicomponent coupling reaction of enolizable ketones with aromatic aldehydes, acetyl chloride and acetonitrile was carried out in the presence of TFA for the preparation of  $\beta$ -acetamido ketones. This method is of great value because of high yields and ease of handling.



일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: II-ORGN.P-315

발표분야: 유기화학

발표종류: 포스터, 발표일시: 목 15:00~17:00

## **EDDA-Catalyzed One-Pot Synthesis of 2-Amino-3-cyano-4H-chromen-4-yl Phosphonate Derivatives in Ethanol**

**KOLLA SRINIVASA RAO, 이용록**

영남대 화학공학부

Three component one-pot reactions of salicylaldehyde with malononitrile or ethyl cyanoacetate and triethyl phosphite were carried out in the presence of EDDA as a catalyst in ethanol for the preparation of biologically active 2-amino-3-cyano-4H-chromen-4-yl phosphonate derivatives. This method is of great value because of its environmentally benign character, high yields, and ease of handling.



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발표종류: 포스터, 발표일시: 목 15:00~17:00

## The Impact of Anions on the Electrocatalytic Activity in Supported Palladium Nanoparticles onto Ionic Liquid-Carbon Nanotube Hybrids for Oxygen Reduction Reaction

신주연, \*김연수, \*이수진, \*\*이종목, 이상기

이화여대 화학/나노과학과 \*이화여대 화학/나노과학과 \*\*이화여대 화학과

A series of supported palladium nanoparticles onto the carbon nanotubes, which were functionalized covalently with imidazolium salt polymer having different anions, Pd/PolyIL(X)-CNT, X = Cl, Br, I, ClO<sub>4</sub>, BF<sub>4</sub>, PF<sub>6</sub>, are prepared to investigate the influence of anions of imidazolium salt on the electrocatalytic activity for oxygen reduction reaction (ORR). The anions of imidazolium moiety significantly impacted on the ORR kinetics in 0.1 M HClO<sub>4</sub> solution. The electronically active surface area results are in a great agreement with the order of the ORR kinetic activity of the supported Pd/PolyIL(X)-CNT (X: Cl > ClO<sub>4</sub> > BF<sub>4</sub> > Br ≈ PF<sub>6</sub> >> I). These results indicate that subtly varied structure of ionic liquid moiety profoundly influence the performance of ionic liquid-CNT hybrid materials, and molecular-level control of interfacial interactions between the support material, catalysts, and electrolytes is important in the design of supported metal nanoparticle catalysts for fuel cells.



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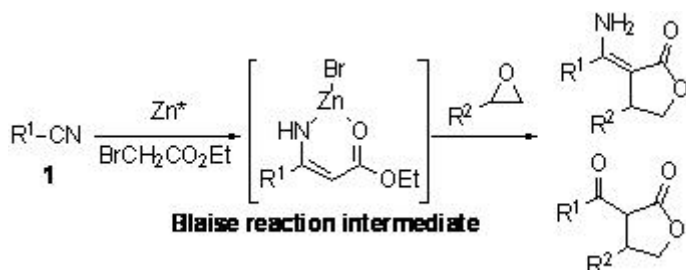
발표종류: 포스터, 발표일시: 목 15:00~17:00

## Tandem synthesis of $\gamma$ -butyrolactone by using the Blaise reaction intermediate

고영옥, \*이상기

이화여대 화학·나노과학과 \*이화여대 화학·나노과학과

The design and implementation of tandem reactions is a challenging facet and become increasingly important in organic chemistry because of their undeniable ability to create complex molecules in a single reaction without the need to isolate intermediate. Recently, we challenged tandem use of the Blaise reaction intermediate, a zinc bromide complex of  $\beta$ -enaminoester, and accomplished the chemoselective nucleophilic addition to anhydrides,[1] terminal alkynes,[2] and propiolates.[3] In present work, we investigated the reactivity of Blaise reaction intermediate towards epoxide ring opening for the synthesis of  $\gamma$ -butyrolactones. References: [1] (a) Chun, Y. S.; Lee, K. K.; Ko, Y. O.; Shin, H.; Lee, S.-g. Chem. Commun. 2008, 5098. (b) Ko, Y. O.; Chun, Y. S.; Park, C.-L.; Kim, Y.; Shin, H.; Ahn, S.; Hong, J.; Lee, S.-g. Org. & Biomol. Chem. 2009, 7, 1132 [2] Chun, Y. S.; Ko, Y. O.; Shin, H.; Lee, S.-g. Org. Lett. 2009, 11, 3414. [3] Chun, Y. S.; Ryu, K. Y.; Ko, Y. O.; Hong, J. Y.; Hong, J.; Shin, H.; Lee, S.-g. J. Org. Chem. 2009, 74, 7556.



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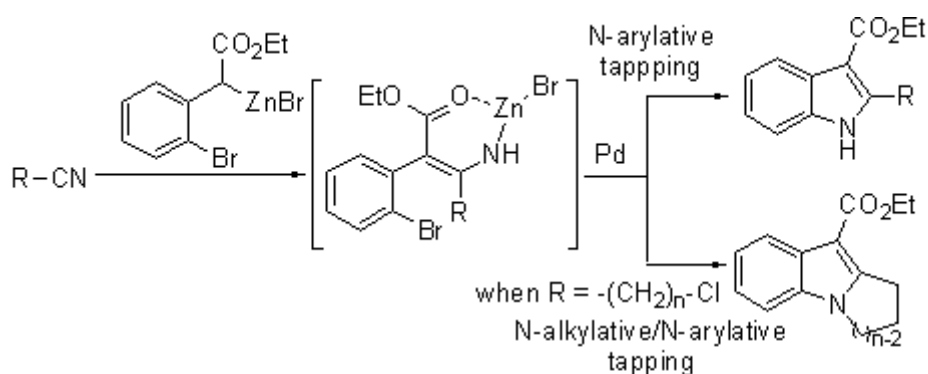
발표종류: 포스터, 발표일시: 목 15:00~17:00

## Pd-Catalyzed Intramolecular Trapping of the Blaise Reaction Intermediate for Tandem One-Pot Synthesis of Indoles from Nitriles

김주현, 박보영, 이상기

이화여대 화학/나노과학과

Indole is a structural component in a vast number of natural products and biologically relevant compounds. To date, numerous elegant approaches have been continuously developed to generate this unique heterocyclic ring moiety. Most of these approaches rely on anilines or amines as nitrogen sources, and therefore the development of new methods for the synthesis of indoles from simple and readily available non-amino compounds is still a subject of interest. As part of our ongoing recent study on the development of tandem reaction by using the Blaise reaction intermediate, we investigated Pd-catalyzed intramolecular N-arylate and N-alkylative/N-arylate trapping of the Blaise reaction intermediate for modular tandem synthesis of Indoles and N-fused indole derivatives from nitriles.



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발표종류: 포스터, 발표일시: 목 15:00~17:00

## Organogelator templates morphology in different solvents and their role in nanostructured silica formation

진종성, 정의덕, \*이미성, \*\*문해경, \*\*\*F.Nawaz Khan

한국기초과학지원연구원 하이테크부품소재연구지원센터 \*부산대 화학과 \*\*한국기초과학지원  
연구원 하이테크소재연구부 \*\*\*Organic Chemistry Division, School of Advance Sciences, VIT  
University, India

The versatile gelation ability of the short chained organogelator was evaluated and found to be gelated in most of organic solvents tested. Scanning electron microscope, (SEM) and Tunnelling electron microscope, (TEM) images of neutral organogels made from different solvents showed that they assembled into plate shaped gelators in ethanol and n-butanol, rod-shaped morphology, in acetonitrile and THF. Similarly 1:1 mixture of neutral and cationic gelators formed different morphologies in different tested solvents. Sol-gel polycondensation of tetraethoxy silane was explored using either individual gels (neutral or cation) or 1:1 mixture of gels. The TEM and SEM images revealed that silica nanotubes of inner diameter 82 nm and an outer diameter 620 nm were obtained from the mixture of neutral and cationic gelator in ethanol, whereas silica nanoparticles were obtained using gels made in other tested solvents.

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발표종류: 포스터, 발표일시: 목 15:00~17:00

## Synthesis and evaluation of [1,2,4]triazolo[3,4- $\alpha$ ] isoquinolines as potential antibacterial agents of resistant strains of Nosocomial pathogen *Acinetobacter baumannii*

**F.Nawaz Khan**, \*진종성, \*정의덕, P.Manivel, \*\*M.R.Rajeswari, \*\*\*이미성, \*\*\*\*문해경

Organic Chemistry Division, School of Advance Sciences, VIT University, India \*한국기초과학지원연구원  
원 하이테크부품소재연구지원센터 \*\*Department of Biochemistry, All India Institute of Medical  
Sciences, India \*\*\*부산대 화학과 \*\*\*\*한국기초과학지원연구원 하이테크소재연구부

Today, the resistance development to antimicrobials is a major problem in confronting organized health care, the widespread use of antibiotics plays a major role in increase of antimicrobial resistance. *Acinetobacter baumannii* organism, an opportunistic, gram negative, cocco-bacillus bacterium account for a large percentage of nosocomial infections like septicemia, bacterimia, pneumonia, wound sepsis, endocarditis, meningitis, and urinary tract infections. The most challenging part of these infections is the extensive antimicrobial drug resistance and emergence of strains that are resistant to all commercially available antibiotics. These strains are invariably multidrug resistant and show resistance against most of the commonly used antibiotics like penicillins, aminoglycosides, cephalosporins, and even fluoroquinolones and the lack of new antimicrobial agents in development. Various 1, 2, 4-triazoles have been extensively explored for their applications in the field of biological and pharmacological activities, including antifungal, bactericidal, anxiolytic, anticonvulsant, or herbicidal and antidepressant activities. Therefore, it was envisaged that chemical entities with 1, 2, 4-triazole might result in compounds with interesting biological activity. In view of this we report herein, a convenient, practical and efficient method for the synthesis of [1, 2, 4]triazolo[3,4- $\alpha$ ]isoquinolines and the antibacterial activity of the triazoles against resistant strains of *Acinetobacter baumannii* was explored.

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## Efficient Synthesis of ( $\pm$ )-Rhinacanthin A, Dehydro $\alpha$ -Lapachone, and $\beta$ -Lapachone

**CHEN YE**, 이용록

영남대 화학공학부

A concise synthesis of ( $\pm$ )-rhinacanthin A is achieved in two steps by epoxidation of dehydro- $\alpha$ -lapachone followed by chemo- and regioselective reduction. Dehydro- $\alpha$ -lapachone was synthesized in two steps starting from 4-methoxy-1-naphthol by ethylenediamine diacetate (EDDA)-catalyzed benzopyran formation and a CAN-mediated oxidation reaction.  $\beta$ -Lapachone was synthesized in three steps from 4-methoxy-1-naphthol by benzopyran formation, catalytic hydrogenation, and Jones oxidation.

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발표종류: 포스터, 발표일시: 목 15:00~17:00

## One-Pot Synthesis of 1,4-Disubstituted 1,3-Diynes via Pd-Catalyzed Decarboxylative Coupling of Propiolic Acids

박지혜, 박언정, 김인수

울산대 화학과

Conjugated 1,3-diynes are very crucial materials in the fields of chemistry, biology and material science, because they have been used in the preparation of natural products, organic and inorganic composites, pharmaceuticals, and  $\pi$ -conjugated polymers as well as the molecular recognition process. Traditional method for the construction of symmetrical or unsymmetrical 1,3-diynes is oxidative homocoupling reactions of terminal alkynes, reported by Glaser, via the treatment of Cu(I) salt in the presence of aqueous ammonia followed by air oxidation. Later related modified methods to improve the disadvantage of the original reaction condition were developed by Eglinton, Hay, Chodkiewicz-Cadiot, and Yu. Pioneering work for the preparation of symmetrical 1,3-diynes using palladium catalysis was reported by Rossi et al. in 1985. Recently, Lei et al. demonstrated new process for the construction of unsymmetrical 1,3-diynes, which includes Ni-catalyzed oxidative coupling of two different terminal alkynes with a high loading of one alkyne partner. However, these methodologies present intrinsic drawbacks, namely the need for prefunctionalization of both coupling partners. For examples, in the case of homocoupling of terminal alkynes, the preparation of terminal alkynes were often required, i.e. via Corey-Fuchs reaction using aldehydes, Fritsch-Buttenberg-Wiechell rearrangement of vinyl bromides, Seyferth-Gilbert homologation using aldehydes, and Sonogashira reaction between haloarenes and metal (Si or Sn)-substituted acetylenes followed by reductive hydrogenation. Moreover, the methods for the synthesis of unsymmetrical 1,3-diynes have required the prefunctionalization to prepare haloalkynes or propiolic acids as well as terminal alkynes. The multi-step syntheses required for the preparation of such substrates can pose additional barriers to their use. Therefore, it is highly desirable to develop more efficient methodologies saving synthetic steps and avoiding waste formation for synthesizing conjugate 1,3-diynes. Herein, we demonstrate direct synthesis of symmetrical 1,4-disubstituted 1,3-diynes from

iodoarenes and propiolic acid via Sonogashira reaction followed by Pd-catalyzed decarboxylative homocoupling. Furthermore, one-pot synthesis of unsymmetrical 1,4-disubstituted 1,3-diynes by cross-coupling of two different 3-substituted propiolic acids is described.





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## Enantioselective Total Synthesis of (+)-Fluvastatin via Catalytic C-C and C-O Bond Formation Reactions

김애진, 문영규, 김미림, 김인수

울산대 화학과

Statins are a class of drugs that lower the cholesterol level in the blood by blocking hydroxymethylglutaryl-coenzyme A reductase (HMG-CoA reductase) in the liver. Statins have become the most frequently prescribed agent for the treatment of hypercholesterolemia due to their effect on reducing the rates of cardiovascular events. Fluvastatin (Lescol<sup>TM</sup>) inhibits the enzyme that reduces 3-hydroxy-3-methylglutaric acid to mevalonic acid, thus blocking cholesterol biosynthesis and lowers low-density lipoprotein cholesterol levels by 20-30% at a daily dose of 20-40 mg. It has also been shown to exhibit antiviral activity against Hepatitis C. Due to their potent pharmacological effects and the unique structural features, statins have attracted considerable attention as powerful synthetic targets. The majority of synthetic approaches have focused on efficient construction of the statins side chain. In 1997, the Novartis research group described a practical asymmetric synthesis of fluvastatin via a highly selective reduction of optically pure  $\delta$ -hydroxyl- $\beta$ -ketoesters with a subsequent Horner-Wadsworth-Emmons reaction. In addition, they developed a manufacturing process for the production of fluvastatin in racemic form. Recently, Hayashi and coworkers reported enantioselective total synthesis of (+)- and (-)-fluvastatin and their analogues through the reaction of an aldehyde with diketene in the presence of  $\text{Ti}(\text{OiPr})_4$  and a chiral Schiff base ligand as the key step. In this paper, we present a new strategy for the asymmetric total synthesis of (+)-fluvastatin, that includes catalytic carbon-carbon bond formations, such as Cu-catalyzed C-3 arylation, Ir-catalyzed asymmetric allylation and Ru-catalyzed intermolecular metathesis, and diastereoselective Michael addition for the preparation of 1,3-syn-diol.

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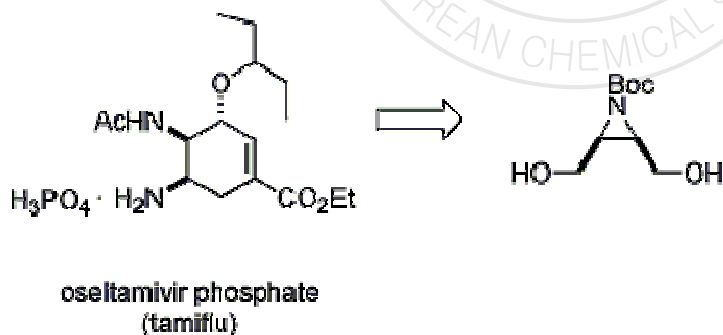
발표종류: 포스터, 발표일시: 목 15:00~17:00

## Synthetic Study toward Oseltamivir (Tamiflu)

강한영, 오홍세

충북대 화학과

Oseltamivir phosphate [Tamiflu(1)] has been the only orally available drug for treatment of human influenza and recent worldwide outbreak of swine flu (H1N1 human flu) and potential threat of avian flu draw an accelerated attention for securing anti-influenza drugs for safeguarding the public health. We have been interested in the synthesis of oseltamivir phosphate [Tamiflu(1)] and have studied an efficient synthetic route starting from 2,3-bis(hydroxymethyl)aziridine. After protection of the aziridine with the Boc group, disymmetrization provided the chiral aziridine which was a key intermediate in our synthetic route. Our effort for the synthesis of oseltamivir [Tamiflu] (1) will be presented.



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발표종류: 포스터, 발표일시: 목 15:00~17:00

## **Bridging of Two Chromophore Molecules for Efficient Photosensitizer in DSSC**

이상희, 김동희, 유수창

군산대 화학과

Chromophore L1 was bridged to KS-5 through phenylenediamine moiety. KS-5 binds to TiO<sub>2</sub> surface very strongly using two anchoring group in TiO<sub>2</sub> based DSSC. The strong binding resulted in increase of adsorbed dye amount on TiO<sub>2</sub>. Multi binding induced rigid non-planar structure which can suppress of aggregation of dye. Also long-term stability could be expected from this strong binding. Another bridging effect is red-shift and broadening in Uv-Vis spectrum. The overall effect gave much higher efficiency of KS-5 ( 6.1 %) compared to corresponding monomer L1( 3.0 %).

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## Synthesis New 1,2-Napthoquinone Derivatives for KAPAS Inhibitor

남기달, \*한민수, \*\*한영휘, 한호규

KIST 생체과학연구부 \*고려대 화학과 \*\*서강대 화학과

신규 작용점의 탐색과 기능 유전자의 발굴 등 혁신적인 방법에 의해 새로운 제초제를 개발하기 위하여 KAPAS 저해 화합물을 발굴하였다. 6-Bromo-2-naphthol 과 2-naphthol 을 각각 출발 물질로 사용하여 1,2-naphthoquinone 유도체를 합성하였다. 합성된 화합물의 KAPAS 에 대한 in vitro 실험 결과와 in vivo 활성 실험을 비교 검토하였다. In vitro 실험에서 작용점/효소를 강력하게 저해하는 물질이 in vivo 시험조건에서 미약한 효과를 나타냈는데 화합물의 작용점까지 침투이행을 증가시키기 위하여 수화제로 만들었더니 괄목할만한 제초활성을 나타냈다. 구조적 결가지 변화에 따른 제초활성의 결과에 의하면 1,2-naphthoquinone 핵에서 side chain 보다는 naphthoquinone 골격이 KAPAS 저해활성에 영향을 주는 것이라고 사료되었다.

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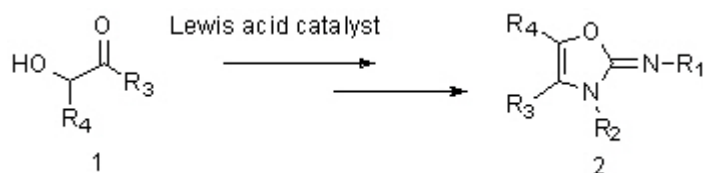
발표종류: 포스터, 발표일시: 목 15:00~17:00

## Novel synthesis of 2-imino-1,3-oxazoline from $\alpha$ -hydroxy-ketones by using Lewis acid catalyst

한민수, \*남기달, 정낙철, \*한호규

고려대 화학과 \*KIST 생체과학연구부

Synthetic methods available for the construction of heterocyclic molecules can be used to affect a number of valuable synthetic transformations. We recently reported a synthesis of 2-imino-1,3-thiazolines which showed antifungal and T-type channel inhibitory activities. 2-Imino-1,3-thiazolines are isoform of 2-amino-1,3-thiazole, which known to be privileged structure in the medicinal chemistry for development of new pharmaceuticals. As an extension of our studies of lead optimization of this series, we now report here a novel synthesis of 2-imino-1,3-oxazolines from the reaction of  $\alpha$ -hydroxy-ketone and diimide in the presence of Lewis acid catalyst. 2-Imino-1,3-oxazolines are oxygen analogue of 2-imino-1,3-thiazolines and expected to show biological activity. While 2-imino-1,3-thiazolines were synthesized by the reaction of  $\alpha$ -halo-ketone and thiourea in quantitative, the oxygen analogue, 2-imino-1,3-oxazolines could not be prepared by the reaction of  $\alpha$ -halo-ketone and urea. The synthetic methodology report here is convenient for preparation of 2-imino-1,3-oxazoline derivatives. We also discuss the regiochemistry of the products.



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발표종류: 포스터, 발표일시: 목 15:00~17:00

## **Piperazine derivatives as novel triple reuptake inhibitors for the treatment of depression**

한영휘, \*남기달, \*\*한민수, 이덕형, \*한호규

서강대 화학과 \*KIST 생체과학연구부 \*\*고려대 화학과

Drugs that interfere with the uptake and metabolism of monoaminergic neurotransmission have been used to treat depression for 40 years. Early medications such as tricyclic antidepressants and monoamine oxidase inhibitors are effective but possess many side effects, that limit their usefulness. Also several serotonin reuptake inhibitors (SSRIs) and selective norepinephrine reuptake inhibitors (SNRIs) were launched in the market. However the low effectiveness, a few side effects are still problem. Therefore, the emergence of new antidepressants are expected. We found out a piperazine derivative which had reuptake inhibitory activity from the library of our compound collection by high throughput screening. Hence we will report a construction of focused library of piperazine derivatives through modification of the structure of the hit compound and their biological activities against SSRI, SNRI and SDRI. Structure-activity relationship will be discussed also.

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발표종류: 포스터, 발표일시: 목 15:00~17:00

## Design, Synthesis and T-type Calcium Channel Inhibitory Activity of 2-Amino-1,3-thiazoles by the Combination of Bio-Active Fragments.

허정희, \*남기달, 정낙철, \*한호규

고려대 화학과 \*KIST 생체과학연구부

2-Amino-1,3-thiazole derivatives which are isoform of 2-imino-1,3- thiazolines were synthesized and their inhibitory activities against T-type  $\text{Ca}^{2+}$  channel were tested to develop of new selective T-type  $\text{Ca}^{2+}$  channel inhibitor. 2-Amino-1,3-thiazole moiety is one of common fragment being in various bio-active pharmaceuticals and it showed relatively low toxicity. Therefore, it called privileged structure. Arylpiperazine and guanidine moieties are also known as one of privileged structure. They have nitrogen atom in the molecule to relate strong hydrogen bond, which would result various biological activities. In the study, novel 2-amino-1,3-thiazole derivatives in which arylpiperazine or guanidine moiety is present in a molecule were designed, synthesized, and constructed the chemical library by combinatorial chemistry method. The synthesized compounds were classified four series depending on the chemical structure. Novel 102 kind of 2-amino-1,3-thiazole derivatives were synthesized. The compounds were screened against T-type  $\text{Ca}^{2+}$  channel, using HEK293 cell (human renal cell carcinoma derived) expressed  $\alpha_{1G}$  at the cell membrane through FDSS6000 attached HTS system and mibefradil was used as a reference compound. The synthetic route and their screening results will be presented.

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발표코드: II-ORGN.P-330

발표분야: 유기화학

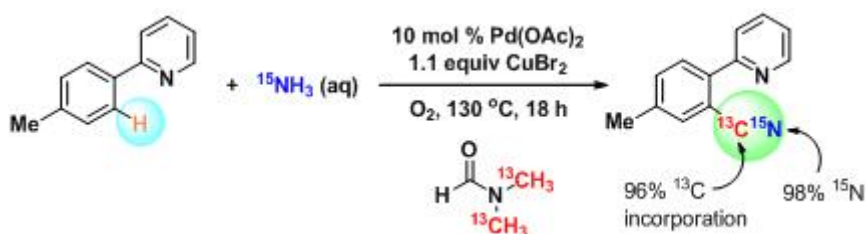
발표종류: 포스터, 발표일시: 목 15:00~17:00

## A New Combined Source of “CN” from N,N-Dimethylformamide and Ammonia in the Palladium-Catalyzed Cyanation of Aryl C–H Bonds

김진호, 장석복

KAIST 화학과

Aromatic nitriles possess versatile utilities and are indispensable not only in organic synthesis but also in chemical industry. In fact, the nitrile group is an important precursor for various functional groups such as aldehydes, amines, amidines, tetrazoles, amides, and their carboxyl derivatives. Representative methods for the preparation of organonitriles with cyanide-containing reagents are the Sandmeyer and Rosenmund-von Braun reactions. Recently, a catalytic route to aryl nitriles has been reported on the basis of the chelation-assisted C–H bond activation or metal-catalyzed cyanation of haloarenes. In those cyanation protocols, the “CN” unit is provided from metal-bound precursors of MCN (M = Cu, K, Na, Zn), TMS-CN, or  $K_3Fe(CN)_6$ . Additionally, it can be generated in situ from nitromethane or acetone cyanohydrin. Herein, we report the first example of generating “CN” from two different, readily available precursors, ammonia and N,N-dimethylformamide (DMF). In addition, its synthetic utility is demonstrated through the Pd-catalyzed cyanation of arene C–H bonds.





일시: 2011년 4월 28~29일(목~금) 2일간

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발표분야: 유기화학

발표종류: 포스터, 발표일시: 목 15:00~17:00

## **Anti-Inflammatory Effects through MTT Assay of Benzophenone-Benzoate Derivatives**

권은미, 전종갑

한림대 화학과

It is generally accepted that benzophenone-benzoate compounds show anti-inflammatory effects due to the arachidonic acid derived from prostaglandin H synthase. It has been known that prostaglandins stimulate inflammation and prohibit lipid decomposition in adipose tissue. Compared to conventional methods such as aspirin through acting as COX inhibitor, nonsteroidal anti-inflammatory drugs (NSAIDs) containing halogen structured compounds were designed to reduce the side effects. Diverse structured benzophenone-benzoate compounds were prepared through DCC coupling, Fries rearrangement by  $AlCl_3$  and  $SN_2$  reaction in overall 3 steps and the synthesized compounds were assayed through MTT assay method.

일시: 2011년 4월 28~29일(목~금) 2일간

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발표분야: 유기화학

발표종류: 포스터, 발표일시: 목 15:00~17:00

## Synthesis of Benzo[b]furan Natural Product Ailanthoidol and their Derivatives for Anti-Inflammatory Activity Test

이나리, 전종갑

한림대 화학과

Ailanthoidol can be isolated from the chloroform-soluble fraction of stem woods of *Zanthoxylum ailanthoides*. While there have been no reports on this compound's biological activities, extracts of the bark and leaves of this tree have been used in folk medicine. The most practical and optimized 5 step reaction procedures including regioselective iodination, Sonogashira coupling with cyclization, Wittig reaction, debenzylation and reduction gave ailanthoidol in 72% overall yield from vanillin. Also, ailanthoidol showed 100% inhibition of NO production at 10 $\mu$ M and 35% inhibition even at 1 $\mu$ M. Ailanthoidol derivatives were prepared with similar method for comparison of their anti-inflammatory effect.

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장소: 제주ICC

발표코드: II-ORGN.P-333

발표분야: 유기화학

발표종류: 포스터, 발표일시: 목 15:00~17:00

## Synthesis of Benzofuran Natural Product and their Indole-type Derivatives

김시준, \*전제호, 전종갑

한림대 화학과 \*한림대 천연의약연구소

Benzofuran is classified into heterocyclic compounds and has many biological activities including insecticidal, fungicidal, anti-microbial, anti-proliferative and antioxidant activities. Egonol, ailanthoidol and XH-14 are belong to the series of benzofuran natural products which have been already prepared. We will synthesize these existing benzofuran natural product and their indole type derivatives. Serotonin and tryptophane are known to be biologically active indole compound. We will prepare indole type ailanthoidol derivatives and compare their anti-inflammatory effects.

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발표분야: 유기화학

발표종류: 포스터, 발표일시: 목 15:00~17:00

## Synthesis of Stilbene Derivatives for Comparison of Antioxidant Activity

정세훈, 전종갑

한림대 화학과

Stilbene is one of the long-known aromatic compounds and exists as cis or trans isomer. Phenolic derivatives of stilbene, especially shows the strong antioxidant activity. The antioxidant activity of stilbene is differ from the type of substituent, position and the structural isomers. Stilbene derivatives were synthesized by existing piceatannol synthesis to compare the antioxidant effect. Antioxidant activities including DPPH, ABTS and tyrosinase inhibitory activity of the stilbene derivatives were compared.

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발표코드: II-ORGN.P-335

발표분야: 유기화학

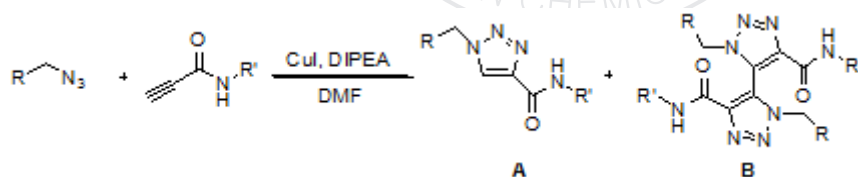
발표종류: 포스터, 발표일시: 목 15:00~17:00

## Unusual reaction of direct Cu(I)-catalyzed 1,3-dipolar cycloaddition to acetylenic amide

장유진, 윤선영, 전홍배

광운대 화학과

C-Carbamoyl-1,2,3-triazoles have been recently attracted to many researchers due to their potent biological activities. So we tried to synthesize the C-carbamoyl-1,2,3-triazoles by 1,3-dipolar cycloaddition with organic azides and acetylenic amides. As a result, when  $\text{CuSO}_4$  and Na ascorbate were used as Cu(I)-catalyst, we obtained only the expected triazole product A. On the other hand, the unexpected product B was obtained as a major product by using direct Cu(I)-catalyst such as CuI, CuBr etc. Herein we present the unusual Cu(I)-catalyzed 1,3-dipolar cycloaddition of acetylenic amides, that afforded the unexpected bistriazole B by using direct Cu(I)-catalysts.



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발표분야: 유기화학

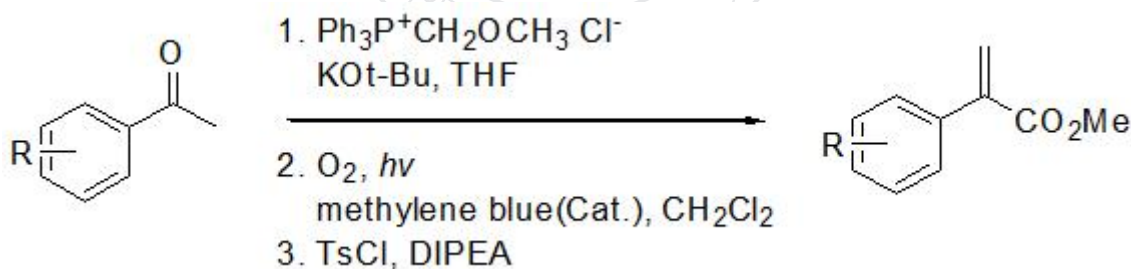
발표종류: 포스터, 발표일시: 목 15:00~17:00

## Synthesis of 2-Arylacrylic esters from aryl methyl ketone via Wittig reaction/singlet oxygen ene reaction

박상준, 김경태, 전홍배

광운대 화학과

2-Arylacrylic esters have been used as an important precursors in organic synthesis due to the high reactivity. We present the synthetic method of 2-Arylacrylic esters from aryl methyl ketone via Wittig reaction/singlet oxygen ene reaction and the tendency of the yield. Wittig reaction to aryl methyl ketone with (methoxymethyl)triphenylphosphonium chloride afforded the methyl enol ether, and then 2-Arylacrylic esters were obtained by singlet oxygen ene reaction to methyl enol ethers. The yields were obtained differently depending on the substituent position.



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발표분야: 유기화학

발표종류: 포스터, 발표일시: 목 15:00~17:00

## Microwave-assistanted diversification of aza-heterocycle by N-arylation

권재관, 엄을균

충남대 화학과

Traditional Ullmann type C-N coupling reaction is required to stoichiometric amounts of copper, harsh condition, long reaction time and strong base. Recently, many paper reported microwave irradiation afforded faster chemical reaction compared with conventional heating reactions. Particularly, microwave reactions showed enormous acceleration of the reaction rate, significant energy savings, as well as high chemical yields and cleaner reactions. So we examined diversification of the heterocycles such as indole, azaindole, pyrazole, and carbazole with microwave-assistant C-N arylation. The heterocycle derivatives are valuable as the precursor of many pharmaceuticals and material science. We will discuss the reaction conditions and application to the material science.

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발표코드: II-ORGN.P-338

발표분야: 유기화학

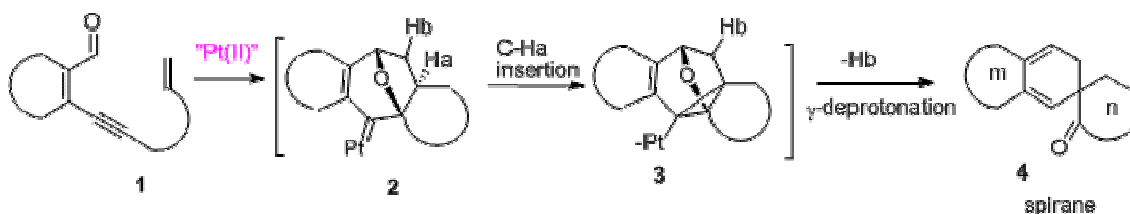
발표종류: 포스터, 발표일시: 목 15:00~17:00

## Synthesis of [m,6,n]-tricyclic spiranes via Intramolecular[3+2] cyclization of Platinum-bound pyrylium with alkenes

이지호, PIAOLANHUA, 박나리, 오창호

한양대 화학과

The cycloaddition reaction is one of the most powerful synthetic tools for the construction of various cyclic compounds. Particularly, intermolecular metal-catalyzed cycloaddition is very attractive because it gives multicyclic compounds from acyclic substrates in one pot. Our group endeavors developed a general and modular route to seven-membered-ring-containing compounds. We have reported divergent behavior of metal-carbene complexes with a Huisgen-type [3+2] cycloaddition between metal-bound pyrylium and a pendant alkene. Our team reported gold-catalyzed [3+2]-cyclization and Rh-catalyzed [3+2]-cycloisomerization of o-alkynylbenzaldehydes with unsaturated bond in 2005. Furthermore, we have observed several unique insertions to Pt-pyrylium complex and generated divergent structural polycycle compounds and reported them. In this study, enynals bearing an olefinic pendant were successfully cyclized via Huisgen-type [3+2] cycloaddition to the tetracyclic Pt-carbene complex as **3** and cycloisomerization of cyclopropane occurred to form the spirane **4** as followed scheme.





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발표분야: 유기화학

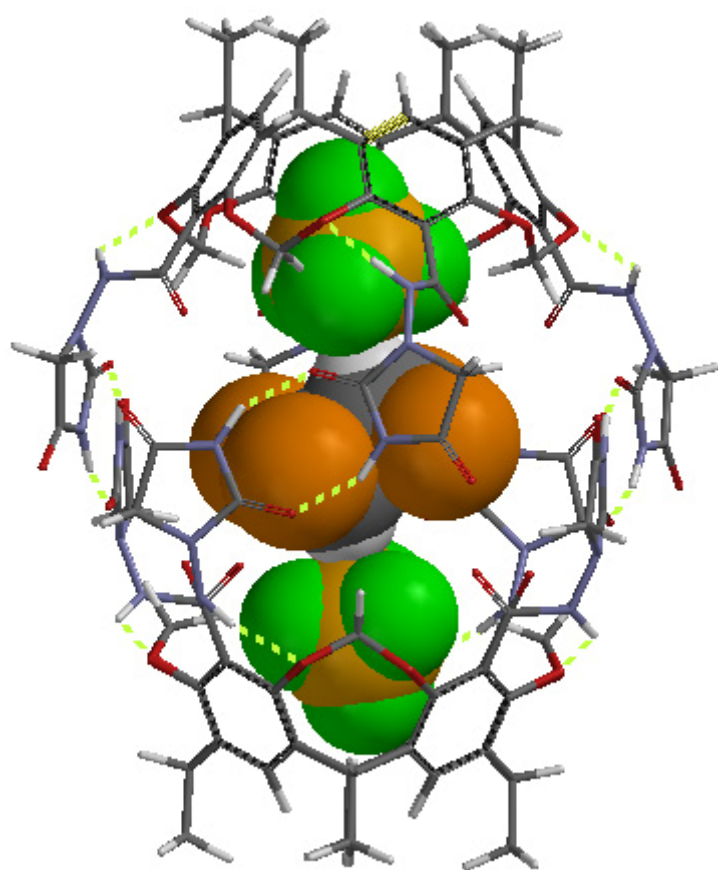
발표종류: 포스터, 발표일시: 목 15:00~17:00

## Resorcin[4]arene-Based amidohydantoin molecular capsule

박연실, 백경수

승실대 화학과

Self-assembling molecular capsules based on noncovalent interactions have attracted considerable interest due to their potentials as molecular storage, sensor, catalysts, or reaction chambers in the field of supramolecular chemistry. The resorcin[4]arene-based amidohydantoin cavitand formed stable molecular capsules in nonpolar solvents by the eight intermolecular imide  $\text{N-H}\cdots\text{O}=\text{C}$  hydrogen bondings, two from each four paired hydantoin moieties, and the four intramolecular  $\text{O-H}_2\text{C-O}\cdots\text{H-N}$  hydrogen bondings on each cavitand. The synthesis and versatile characteristics of this amidohydantoin molecular capsule toward anionic and neutral guests will be presented.



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발표분야: 유기화학

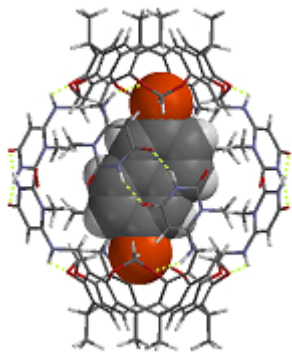
발표종류: 포스터, 발표일시: 목 15:00~17:00

## Cavitand-based Molecular Capsule with a Uracil Motif

서성종, 박연실, 백경수

승실대 화학과

Molecular capsules through multiple hydrogen bonds have been mainly based on complementary assemblies of two cavitands and provide an isolated nanospace. Guest molecules encapsulated in this space show unique properties. Cavitands having four uracil moieties on the upper rim of its resorcin[4]arene structure formed stable molecular capsules through self-complementary hydrogen bondings of imide groups in uracil moieties. The synthesis and versatile characteristics of this uracil molecular capsule toward anionic, cationic, and neutral guests will be presented.



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발표코드: II-ORGN.P-341

발표분야: 유기화학

발표종류: 포스터, 발표일시: 목 15:00~17:00

## Design and Synthesis of a Conjugated Macrocycle Based on the Unique Conformational Bias of Dibenzyl Meldrum's Acid Moieties

송영지, \*이승윤, 문봉진

서강대 화학과 \*한국생산기술연구원 그린공정연구부

Generally, intermolecular coupling methodology to form macrocycles suffers from poor yield, because the cyclization process usually accompanies more significant entropy loss than oligomerization. However, if one can devise a monomer that is already conformationally pre-oriented for the coupling reaction to form a macrocycle, the cyclization yield should be enhanced. In our recent study, we noticed that 5,5-dibenzyl Meldrum's acid has a specific and rigid three-dimensional arrangement where the two phenyl rings surround the Meldrum's acid unit in both sides with high rigidity. It was envisioned that this unique conformational bias can be utilized for building a conjugated macrocycle in high yield. We designed a monomer that has two phenyl acetylene units within a 5,5-dibenzyl Meldrum's acid unit and quickly achieved the monomer synthesis. Triple bond contributes to the rigid structure of the monomer and additional unique photophysical and electrical properties. Finally an attempt to assemble the corresponding macrocycle by Sonogashira coupling yielded the desired product in high yield.

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장소: 제주ICC

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발표분야: 유기화학

발표종류: 포스터, 발표일시: 목 15:00~17:00

## Substituent Effect of the Benzyl Radicals in the Free Radical Initiated Peptide Sequencing (FRIPS)

박혜연, 성연미, 오한빈, 문봉진

서강대 화학과

Mass spectrometry (MS) is one of the most powerful tools in peptide sequencing. Among many methods for characterizing gas-phased peptides, the free radical initiated peptide sequencing (FRIPS), has been under spotlight because the method provides the mass-fragmentation patterns similar to those obtained by the electron collision dissociation (ECD) method under collision induced dissociation (CID) conditions. Generally the FRIPS technique requires introduction of a free-radical generating group into a peptide chain so that a radical species can be generated under CID conditions. We have recently reported a new FRIPS reagent based on (2,2,6,6-tetramethylpiperidine-1-oxy)-(TEMPO) capped benzyl groups and demonstrated that it worked successfully. As an extension of the study, we have synthesized a series of the reagents with different substituents at the para-position and obtained FRIPS data of various peptides using these reagents in series. In this poster will be discussed the relationship between the constitution of the radical and the peptide fragmentation pattern.

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발표분야: 유기화학

발표종류: 포스터, 발표일시: 목 15:00~17:00

## Synthesis of structurally diverse perylenequinone derivatives

김범태, \*방성준, \*한인철, \*\*조익수, \*\*황기준

전북대 생리활성물질연구소, 생리활성소재과학과 \*전북대 생리활성소재과학과 \*\*전북대 화학과

As one of the alternative photosensitizers to Photofrin II, naturally occurring perylenequinones have gained considerable attention due to their excellent photophysical and photochemical properties. However, there has not been reported much on the preparation of a variety of structural modified derivatives and the structure-activity relationship, because of the difficulty to prepare them in the aspect of the very lengthy and tricky synthetic pathway. In this report, one synthetic approach to the efficient and economic construction of perylenequinone core is presented, and the synthetic effort to prepare final active forms of perylenequinones is also demonstrated.

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발표코드: II-ORGN.P-344

발표분야: 유기화학

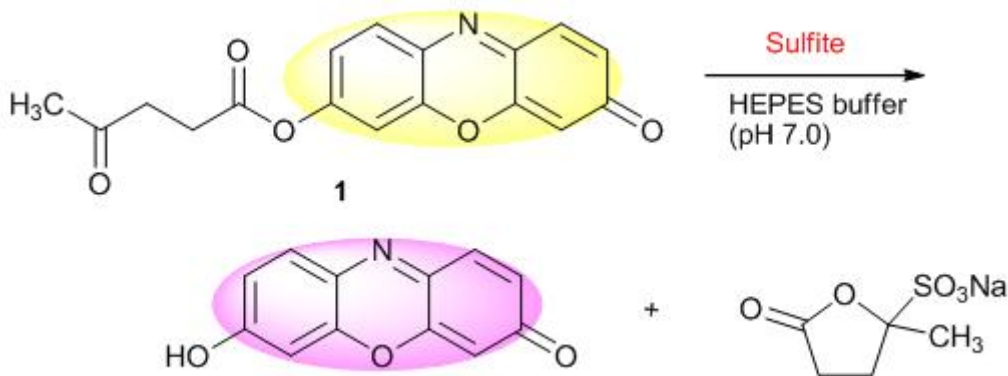
발표종류: 포스터, 발표일시: 목 15:00~17:00

## Chromogenic and Fluorogenic Signaling of Sulfite by Selective Deprotection of Resorufin Levulinate

최명길, 황지영, 어수영, 문정옥, 장석규

중앙대 화학과

A new sulfite-selective signaling system based on resorufin was investigated. A resorufin levulinate **1** exhibited prominent 'OFF-ON' type fluorescence behavior and solution color change from yellow to pink. The signaling is based on the selective deprotection of levulinate groups of probe induced sulfite, which resulted in chromogenic and fluorogenic signaling. Probe **1** also a pronounced selectivity over other delegate anion with a detection limit of  $4.9 \times 10^{-5}$  M (4.0 ppm) in a 98% aqueous acetonitrile solution.



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발표분야: 유기화학

발표종류: 포스터, 발표일시: 목 15:00~17:00

## Dual Signaling of Hypochlorous Acid by Selective Deprotection of pyrene derivative

황지영, 최명길, 문정옥, 장석규

중앙대 화학과

A new hypochlorous acid(HClO)-selective signaling system based upon pyrene derivative was investigated. The pyrene derivative exhibited a prominent 'OFF-ON' type fluorescence signaling based on the selective deprotection reaction by hypochlorous acid. It also showed very efficient HClO-selective signaling in the presence of common alkali and alkaline earth metal ions as well as various anions. The detection limit for hypochlorous acid was approximately 0.97  $\mu\text{M}$  in a 50% aqueous acetonitrile solution(v/v). Furthermore, HClO-selective signaling was detectable when excess amount of hydrogen peroxide was coexistent.



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발표분야: 유기화학

발표종류: 포스터, 발표일시: 목 15:00~17:00

## Analysis of Chlorine Substituent Effect on Benzoyl Chloride derivatives by Grunwald-Winstein Equations.

박경호, \*경진범, 이용우, \*\*고한중, \*\*\*Dennis N. Kevill

한양대 응용화학과 \*한양대 과학기술대학 응용화학과 \*\*전주교육대 과학교육과 \*\*\*Northern Illinois University, USA

Rates of solvolysis reactions of 2,6- and 2,4-Dichlorobenzoyl chlorides and 2,4,6-trichlorobenzoyl chloride were determined and analyzed by the Grunwald-Winstein equation. 2,6-Dichlorobenzoyl chloride shows the typical unimolecular mechanism based on the steric hindrance which is due of blocking the reaction center by two chloride substituents on both ortho positions of benzene ring. 2,4,6-Trichlorobenzoyl chloride also shows unimolecular mechanism, however, this result contains the increasing of bimolecular character than the former compound. This comparison can be considered as the effect of chlorine substituent on para-position. Similarly, a comparison between 2,6- and 2,4-dichlorobenzoyl chlorides allows the added steric effect of introducing the second chlorine substituent at the ortho position to be evaluated.

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발표분야: 유기화학

발표종류: 포스터, 발표일시: 목 15:00~17:00

## One-Pot Synthesis of 5-Hydroxy-( $\alpha$ -Aminomethylene)benzofuran-2(3H)-ones via Tandem Blaise-Nenitzescu Type Reaction

전유성, 이준희, \*이상기

이화여대 화학·나노과학과 \*이화여대 화학·나노과학과

Owing to the nature of minimization of synthetic steps and concurrent maximization of molecular complexity, tandem bond formations are highly attractive in modern synthetic design. Indeed, the device and implementation of tandem reactions is a challenging facet and has become increasingly important in organic synthesis. We were intrigued by the possibility that the Blaise reaction intermediate, a zinc bromide complex of  $\beta$ -enaminoester of the type 2, could be used in tandem reactions. Recently, we have demonstrated that the Blaise reaction intermediate can react, as a carbon-nucleophile, with various electrophiles such as anhydrides, terminal alkynes and propiolates, affording  $\alpha$ -acyl- and  $\alpha$ -vinylated  $\beta$ -enaminoesters and 2-pyridones, respectively. To further expand the capacities of the Blaise reaction intermediate to the synthesis of versatile and difficultly accessible architecture, we investigated the cascade reaction of 2 with 1,4-benzoquinone as an electrophile. In contrast to the classical Nenitzescu reaction in which the condensation of  $\beta$ -enaminoesters 3 with 1,4-benzoquinone provides 3-carboxylated 5-hydroxyindoles 4, the tandem one-pot reaction between 2 and 1,4-benzoquinone affords 5-hydroxy-( $\alpha$ -aminomethylene)-benzofuran-2(3H)-ones 5 in excellent yields.



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발표분야: 유기화학

발표종류: 포스터, 발표일시: 목 15:00~17:00

## Synthesis of 2,5-Substituted 6-Azaindole from Aziridines via intramolecular Cyclization

김준희, 이호규, 이원구, \*하현준

서강대 화학과 \*한국외국어대 화학과

Azaindoles and substituted azaindoles can be found in various natural products and the importance of azaindole derivatives is also found in pharmacologically and biologically active substances. We were interested in the new strategy for the efficient preparation of 2,5-substituted 6-azaindoles from the sequential reactions including a new pyrrole synthesis followed by subsequent intramolecular cyclization of the azide into internal acetylenic unit to provide azaindoles



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발표분야: 유기화학

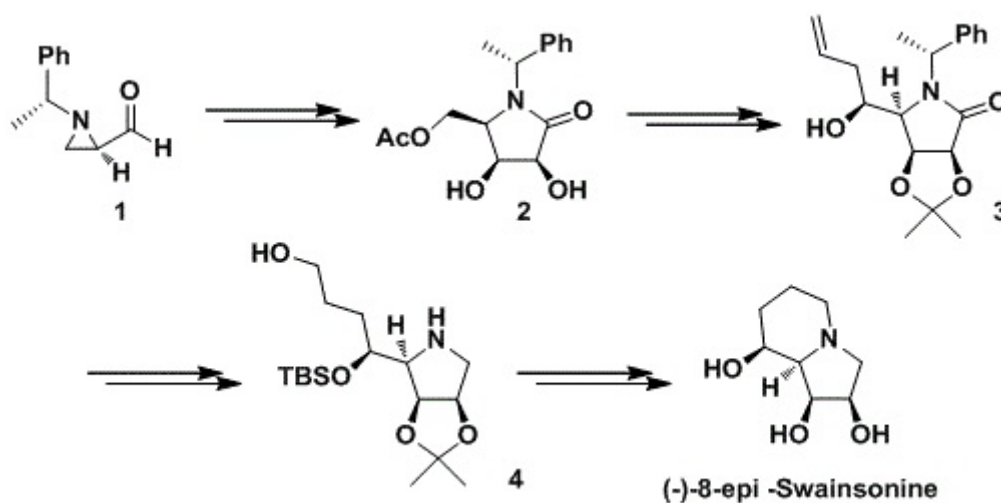
발표종류: 포스터, 발표일시: 목 15:00~17:00

## An Efficient Synthesis of (-)-8-epi -Swainsonine from Chiral Aziridine 2-Carboxylaldehyde

이백경, 김직녀, 이원구, \*심태보

서강대 화학과 \*KIST 생체과학연구본부

A highly enantioselective synthetic approach to 8-epi-D-swainsonine synthesis has successfully been developed starting from chiral aziridine. Enantiomerically pure aminosugar 2 was synthesized via Sharpless asymmetric dihydroxylation on chiral methyl cis-3-aziridin-2-yl-acrylates, followed by the regioselective ring opening of aziridine and acid catalyzed cyclization. By taking advantage of Brown asymmetric allylation, Compound 2 was stereospecifically transformed into the chiral allylic alcohol 3 which underwent hydroboration along with a simultaneous lactam reduction reaction and subsequently debenzoylation to afford the chiral aminoalcohol 4. Compound 4 was submitted to tandem bromination / intramolecular cyclization to furnish the desired final compound, 8-epi-D-swainsonine.



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발표분야: 유기화학

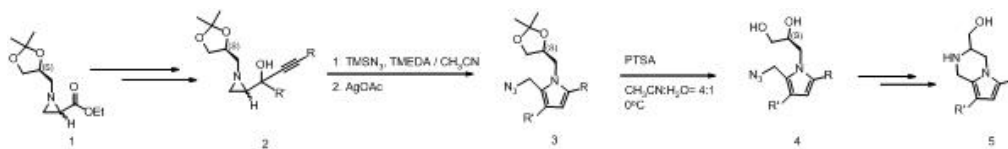
발표종류: 포스터, 발표일시: 목 15:00~17:00

## Asymmetric Synthesis of 6,8-Disubstituted-1,2,3,4-Tetrahydropyrrolo[1,2-a]pyrazin-3-yl)methanols from Chiral Aziridines

강경연, 장만수, 이원구, \*하현준

서강대 화학과 \*한국외국어대 화학과

A number of compounds having 1,2,3,4-tetrahydropyrrolo-[1,2-a]-pyrazine heterocycle have been reported. These compounds can be used as precursors in the synthesis of useful physiologically or psychologically active drugs. Thus, we were interested in the synthesis of enantiomerically pure 1,2,3,4-tetrahydropyrrolo[1,2-a]pyrazine derivatives starting from chiral aziridines. Chiral precursor 1 was generated from the chiral amine, which was obtained from D-mannitol. Depends on the type of lithium agents used on the compound 1 for the generation of tertiary alcohol 2, various kinds of 2-(azidomethyl)-1-((2,2-dimethyl-1,3-dioxolan-4-yl)methyl)-1H-pyrrole 3, differing substituents on 3 and 5 positions were generated. The acetone deprotection of the pyrrole 3 followed by reductive cyclization of the azide provided the desired product 5. Various kinds of alkyl, aromatic substituents on 6, 8 position of 5 were introduced using different lithium agents on the compound 1.



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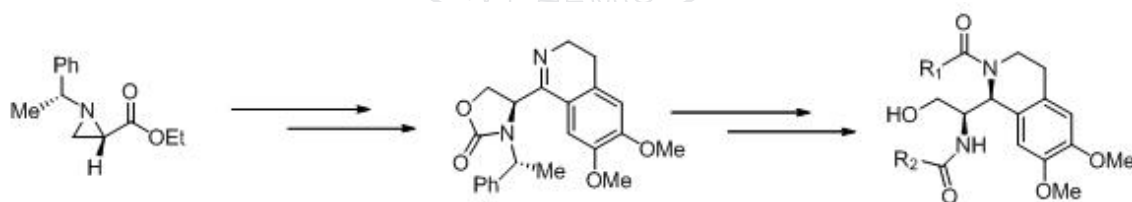
발표종류: 포스터, 발표일시: 목 15:00~17:00

## An Efficient Synthesis of Enantiomerically Pure 1,2,3,4-Tetrahydroisoquinolines Containing $\beta$ -Hydroxyamide Scaffold from a Chiral Aziridine

이규명, 심연수, 이원구, \*하현준

서강대 화학과 \*한국외국어대 화학과

Substituted tetrahydroisoquinolines can be found in many pharmaceutically important molecules. Therefore, we were interested in the synthesis of enantiomerically pure 1,2,3,4-tetrahydroisoquinolines starting from a chiral aziridine. The synthesis of enantiomerically pure 6,7-dimethoxy-1,2,3,4-tetrahydroisoquinoline was successfully achieved via Bischler-Napieralski isoquinoline synthesis from an oxazolidine-4-carboxamide. Various substituents were attached to the two nitrogens of the 1,2,3,4-tetrahydroisoquinoline including  $\beta$ -hydroxyamide after stereoselective reduction of the imine.



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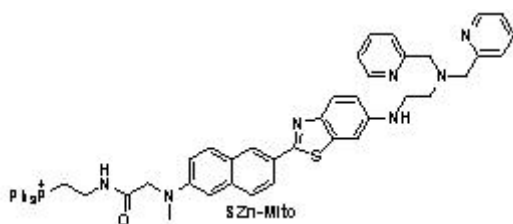
## A Mitochondrial-Targeted Two-Photon Probe for Zinc Ion

MASANTA GOUTAM, \*임창수, \*\*김형중, \*조봉래, \*\*김환명

아주대 분자과학기술연구센터 \*고려대 화학과 \*\*아주대 에너지시스템학부

$Zn^{2+}$  modulates brain excitability and plays a key role in synaptic plasticity. In the brain, ~5-20% of total  $Zn^{2+}$  is stored in presynaptic vesicles with the highest intracellular free  $Zn^{2+}$  ( $[Zn^{2+}]_i$ ) being found in the hippocampus. Recent studies suggest that mitochondrias take up evoked  $[Zn^{2+}]_i$  rise, thereby controlling the  $[Zn^{2+}]_i$  homeostasis. To understand the physiology of  $Zn^{2+}$  in the brain, it is crucial to monitor  $[Zn^{2+}]_m$  in the intact brain tissues.

Herein, we report a two-photon probe (SZn-Mito) for mitochondrial zinc ions ( $[Zn^{2+}]_m$ ). This probe shows a 7-fold two-photon excited fluorescence enhancement in response to  $Zn^{2+}$ , dissociation constant ( $K_d^{TP}$ ) of  $(3.1 \pm 0.1)$  nM, pH insensitivity in the biologically relevant range, and can detect  $[Zn^{2+}]_m$  in a rat hippocampal slice at a depth of 100-200  $\mu m$  without interference from other metal ions by using two-photon microscopy.





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발표종류: 포스터, 발표일시: 목 15:00~17:00

## Dual-Color Two-Photon Probes for Autophagy Imaging

박선근, \*임창수, \*조봉래, 김환명

아주대 에너지시스템학부 \*고려대 화학과

Autophagy is a cellular pathway to degrade aged-organelles through the activities of lysosome. Autophagy plays critical roles in many physiological and pathological processes. Old, damaged, or surplus mitochondria are the major targets for autophagy. To understand these functions, dual-color imaging with a pair of one-photon (OP) fluorescent probes for mitochondria and lysosomes have been utilized. Herein, we report that a pair of two-photon (TP) fluorescent probes for lysosome and mitochondria. These probes emit strong TP excited fluorescence in the different spectral ranges and can simultaneously detect the activities of lysosome and mitochondria in live cells and tissues for a long period time.

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발표종류: 포스터, 발표일시: 목 15:00~17:00

## Development of Two-Photon Turn-on Probes for Imaging Zinc Ion

백나영, \*MASANTA GOUTAM, 김환명

아주대 에너지시스템학부 \*아주대 분자과학기술연구센터

Zinc ion is the second most abundant d-block metal ion in human brain and is an active component in enzymes and proteins. It plays crucial roles in the survival, growth, and metabolism of unicellular and multicellular organisms. To understand its role in physiology, it is crucial to visualize the distribution and transport of  $\text{Zn}^{2+}$  in live cells and intact tissues. For this purpose, we developed two-photon fluorescent (TPF) turn-on probes for imaging of intracellular free zinc ion. These probes show 35~70-fold TPE fluorescent enhancement in response to  $\text{Zn}^{2+}$ , with dissociation constant ( $K_{\text{dTP}}$ ) of 1.4~7.4 nM, respectively. They are highly selective towards  $\text{Zn}^{2+}$  and pH insensitive in the biologically relevant range. These novel probes can selectively detect  $[\text{Zn}^{2+}]_{\text{i}}$  in living specimen.

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발표분야: 유기화학

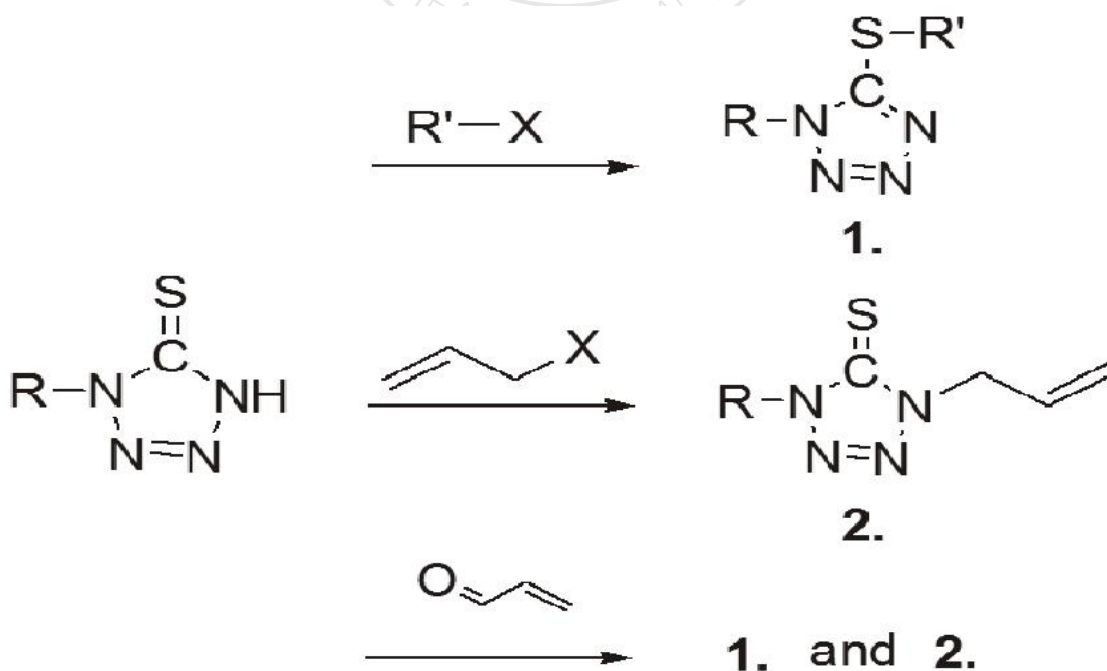
발표종류: 포스터, 발표일시: 목 15:00~17:00

## Nucleophilic Addition Reactions of 1-Substituted-1H-tetrazole-5(4H)-thiones

이제우, 김희정, \*경영수

강릉대 화학신소재학과 \*강릉대 화학과

The reaction of 1-substituted-1H-tetrazole-5(4H)-thiones with various nucleophiles such as alkyl halide, allyl halide,  $\alpha,\beta$ -unsaturated aldehyde under basic condition gave S- and N-substituted derivatives depend on the nucleophile. Addition reactions with alkyl halide, S-substituted derivatives were obtained as a sole product, While allyl halide gave only N-substituted product. The other nucleophile such as  $\alpha, \beta$ -unsaturated aldehyde gave mixture of S- and N-substituted derivatives. Molecular structure of S- and N-substituted derivatives were confirmed by NMR.



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발표코드: II-ORGN.P-356

발표분야: 유기화학

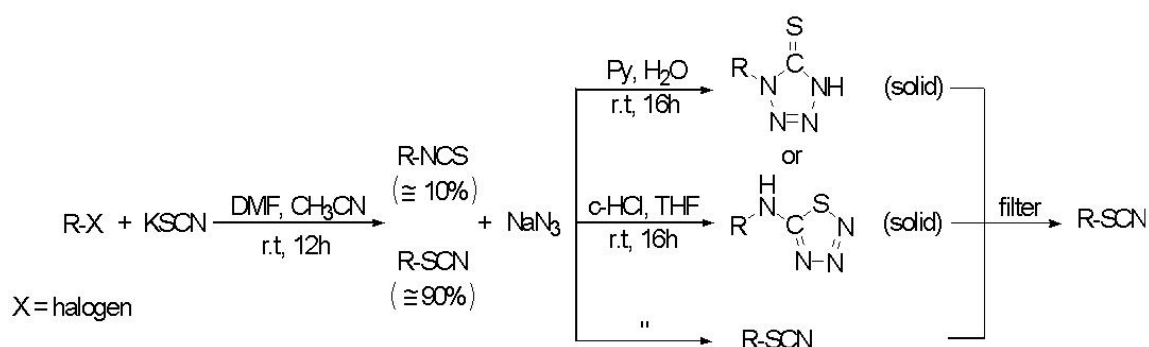
발표종류: 포스터, 발표일시: 목 15:00~17:00

## Selective Reaction of Thiocyanates from Isothiocyanates with Azide ion.

김희정, 이제우, \*경영수

강릉대 화학신소재학과 \*강릉대 화학과

An important method for preparing thiocyanates is substitution of a halogen in halides by the thiocyanate ion. However thiocyanate anion is ambidentate, the reaction can give mixture of thiocyanates and isothiocyanates. It is very difficult to separate thiocyanates and isothiocyanates for the similar physical properties of both compounds. The reaction of isothiocyanates with sodium azide gives selectively N-substituted-1,2,3,4-thiatriazol-5-amines and 1-substituted-1H-tetrazole-5(4H)-thiones depends on the reaction condition. However the reaction of thiocyanates with same condition showed no reactivity. We applied these reactivity to separate thiocyanates exclusively from isothiocyanates via filtration of solid precipitation of tetrazole and thiatriazole derivatives.



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발표분야: 유기화학

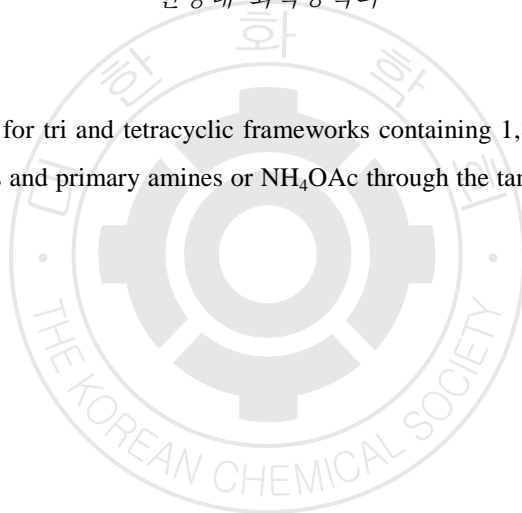
발표종류: 포스터, 발표일시: 목 15:00~17:00

## Synthesis of Tetrahydrobenzo[*b*][1,8]naphthyridine and Tetrahydrodibenzo[*b,g*][1,8]naphthyridine Derivatives

장승순, 안상현, 이기정

한양대 화학공학과

A simple synthetic method for tri and tetracyclic frameworks containing 1,8-naphthyridine moiety from the Baylis–Hillman acetates and primary amines or  $\text{NH}_4\text{OAc}$  through the tandem  $\text{S}_{\text{N}}2'$ – $\text{S}_{\text{N}}\text{Ar}$  reaction has been described.



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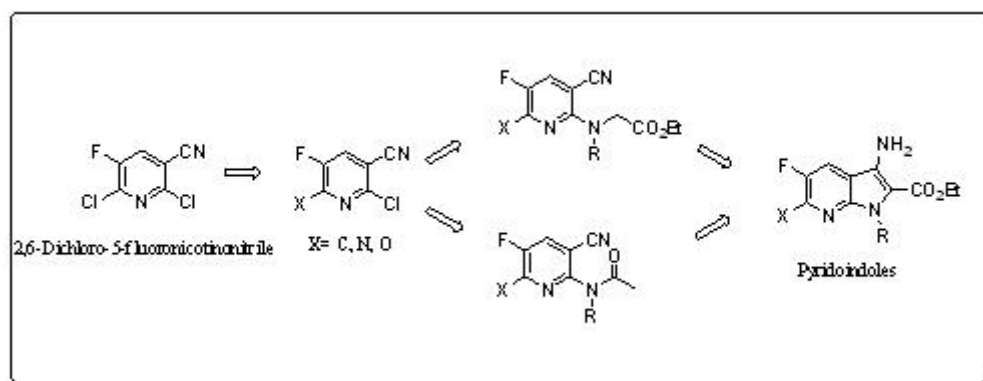
발표종류: 포스터, 발표일시: 목 15:00~17:00

## Design and Synthesis of Modified Pyridoindole Systems from 2,6-Dichloro-5-fluoronicotinonitrile Derivatives

임동희, 김재기, \*정지선, 오창호

한양대 화학과 \*한양대 자연과학대학 화학과

Pyridoindole compounds are important in both the biological and material sciences. More specifically, several substituted 2,6-Dichloro-5-fluoronicotinonitriles are important intermediates in the synthesis of heteroaromatic molecules and biologically active compounds. In the course of our recent medicinal chemistry efforts, we designed and pursued a novel series of compounds built upon intermediates for Pyridoindole system. As a result, our efforts shows that the development of efficient a synthetic scheme to obtain excellent bio-activities of this class of compounds .



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발표분야: 유기화학

발표종류: 포스터, 발표일시: 목 15:00~17:00

## New Intramolecular Hydroarylation

엄다한, 서석진, 이필호

강원대 화학과

Development of an efficient cyclization method is very important for the biological and pharmaceutical applications. Metal-catalyzed hydroarylation of arene-alkynes has attracted much attention in the pivotal areas of synthesis of conjugated aromatic compound in an atom-economical manner. Moreover, the importance of its intramolecular reaction has been widely recognized as a feasible approach to cyclic vinylarene frameworks. In this poster, we describe efficient intramolecular hydroarylation with alkynyl arene.

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발표분야: 유기화학

발표종류: 포스터, 발표일시: 목 15:00~17:00

## Novel Meerwein-Ponndorf-Verley Reduction

엄다한, 이재영, 이필호

강원대 화학과

Among the various methods for reducing carbonyl groups, the Meerwein-Ponndorf-Verley (MPV) reduction is a long-established and still important method in organic synthesis. The MPV reduction of ketones and aldehydes uses inexpensive and environmentally friendly iPrOH as a hydride source and aluminum alkoxides as catalysts. However, aluminum-mediated MPV reduction is limited due to its requirement of a stoichiometric amount of the aluminum alkoxide catalyst and sometimes low yields. Recently, we report efficient MPV reduction of aldehydes to produce alcohol in good to excellent yields.



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발표분야: 유기화학

발표종류: 포스터, 발표일시: 목 15:00~17:00

## Isomerization of Kinetic Enol Derivatives

강동진, 최수빈, 이필호

강원대 화학과

The more stable thermodynamic enol derivatives from unsymmetrical ketones normally predominate under thermodynamic conditions but do not form exclusively, which is a serious problem in organic synthesis. Thus, the preparation of thermodynamic enol derivatives with high selectivity is of synthetic importance and still a very challenging problem. We have developed an efficient metal-catalyzed isomerization of kinetic enol derivatives, such as enol phosphates, enol acetates, enol benzoates, and enol sulfonates, to thermodynamic isomers. In addition, less stable vinyl sulfides can be smoothly isomerized to more stable ones in the presence of metal-catalyst in dichloroethane.

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## Addition of Diphenyl Phosphate to Alkynes Catalyzed by Gold and Its Application to Isomerization

김상혁, 이도형, 이필호

강원대 화학과

Conversion of carbonyl compounds into enol phosphates is of a great synthetic importance since enol phosphates are versatile intermediates which undergo various synthetically useful transformations. The major issue in this transformation is selectivity. Especially, the more substituted thermodynamic enol derivatives from unsymmetrical ketones normally predominate under thermodynamic conditions but do not form exclusively, which is a serious problem in organic synthesis. Thus, the preparation of thermodynamic enol phosphates as highly pure form is of synthetic importance and still a very challenging problem. We have developed the hydrophosphorylation reaction of alkynes using diphenyl phosphate in the presence of  $\text{Ph}_3\text{PAuCl}/\text{AgPF}_6$  to afford the kinetic enol phosphates. Whereas the reaction using  $(\text{C}_6\text{F}_5)_3\text{PAuCl}/\text{AgOTf}$  gave the thermodynamic enol phosphates as highly pure forms. In addition,  $(\text{C}_6\text{F}_5)_3\text{PAuOTf}$  proved to be highly efficient catalyst for the isomerization of kinetic enol phosphates into thermodynamic isomers.

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## Preparation of Ethyl 2-Aryl 2,3-Alkadienoates via Palladium-Catalyzed Selective Cross-Coupling Reactions

강동진, 김진식, 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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발표분야: 유기화학

발표종류: 포스터, 발표일시: 목 15:00~17:00

## Synthesis of Di-, Tri-, and Tetrasulfides through Multifold Carbon-Sulfur Cross-Coupling Reactions with Indium Tri(organothiolates) in a One-Pot Procedure

박영철, 서정민, 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. Over the last decades, transition metals, such as Pd, Ni, Cu, and Fe, have been applied in carbon-sulfur cross-coupling reactions, leading to the effective formation of sulfides with a wide range of functional group tolerance. We found that indium tri(organothiolates)  $(RS)_3In$  were atom-efficient nucleophilic coupling partners in Pd-catalyzed carbon-sulfur cross-coupling reactions. In these reactions, indium organometallics such as triorganoindium and indium tri(organothiolate) transfer all three organic groups to electrophiles. These results have stimulated our interest in its application to multifold carbon-sulfur cross-coupling reactions in a one-pot procedure. Herein, efficient multifold and sequential Pd-catalyzed carbon-sulfur cross-coupling reactions are described with indium tri(organothiolates) in a one-pot procedure, producing di-, tri-, and tetrasulfides.

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발표분야: 유기화학

발표종류: 포스터, 발표일시: 목 15:00~17:00

## Efficient Conia-ene Reaction

박영철, 오수성, 이필호

강원대 화학과

The importance of cyclopentanoid natural products continues inspire the development of methods for the synthesis of 5-membered rings. The intramolecular ene reaction of unsaturated ketones and aldehydes, namely, the Conia-ene reaction, is an important strategy; however, the high temperature needed severely limits its synthetic utility. The utility of this cyclization methodology has been significantly expanded in recent years by the use of 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. A catalytic version of the Conia-ene reaction that proceeds at ambient temperatures and under neutral conditions would dramatically increase the utility of this reaction. Herein, we report an efficient synthetic method of 5-membered rings via new Conia-ene reaction.

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발표분야: 유기화학

발표종류: 포스터, 발표일시: 목 15:00~17:00

## Cyclization of 2-Azetidinone Derivatives

모준태, 박성국, 이필호

강원대 화학과

Carbapenem antibiotics are often the last resort in the treatment of infections caused by bacteria resistant to penicillins and cephalosporins. Although many carbapenems are natural products, they are produced by multistep total synthesis for medicinal use. Studies of carbapenem biosynthesis are of significant interest as they may enable the development of more efficient biochemical production methods. There are several notable reports on the construction of carbapenem skeletons with palladium, silver, and gold catalyzed intramolecular cyclization. We describe that treatment of 2-azetidinone derivatives with various metals produced the bicyclic  $\beta$ -lactam products, carbapenem skeletons, in good yields.

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발표분야: 유기화학

발표종류: 포스터, 발표일시: 목 15:00~17:00

## Development of Synthetic Method for Indolizine Dervatives

모준태, 이의철, 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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발표분야: 유기화학

발표종류: 포스터, 발표일시: 목 15:00~17:00

## Efficient Synthetic Method of Alkenyl Triflate

박상준, 손익환, 이필호

강원대 화학과

Alkenyl triflates are important building blocks in organic synthesis, as intermediates for C-C bond formation by Pd-catalyzed coupling reactions. Surprisingly enough, only two routes are used to prepare these important intermediates and they are mainly obtained from ketones. Deprotonation of the ketone and further trapping of the so-formed enolate by a triflating agent leads to alkenyl triflates. They can also be produced by direct triflation of the ketone to yield a gem-bis(triflate) intermediate, followed by elimination with a bulky base. The main problem associated with these methods is two-step reaction and costly reagents. In this poster, we describe efficient synthetic method of alkenyl triflate.



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발표코드: II-ORGN.P-369

발표분야: 유기화학

발표종류: 포스터, 발표일시: 목 15:00~17:00

## Palladium-Catalyzed Cross-Coupling Reaction of Aryl Iodide Using OrganoIndium Reagent

박상준, 조재영, 이필호

강원대 화학과

Enynes have been receiving considerable attention in organic synthesis. The famous antibiotics such as calicheamicine and dynemicin have conjugated enyne moiety as the essential structure for their biological activities. Enynes are also very important compounds in synthetic organic chemistry. Enynes are fundamental building blocks in organic synthesis. The synthesis of enynes has received special attention in these days and some methods have already been published. However, the synthetic method of enynes through cross-coupling reactions is still rare in organic reactions. So, we are interested in the synthesis of enynes and have developed method a variety of enynes through Pd-catalyzed cross-coupling reactions.

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발표코드: IV-ORGN.P-221

발표분야: 유기화학

발표종류: 포스터, 발표일시: 금 15:00~17:00

## **Pd-Catalyzed Carbonylative and Decarboxylative Reaction of Aryl Iodides and Alkynyl Carboxylic Acids**

박아별, 정은혜, 이선우

전남대 화학과

Alkynyl carboxylic acids reacted with aryl iodides under a CO atmosphere in the presence of a palladium catalyst to produce  $\alpha,\beta$ -alkynyl aryl ketones in good yields. The maximum turnover number was 16800. The desired carbonylative coupling was formed from phenyl propiolic acid without any formation of a noncarbonylative coupling product in the absence of CuI. However, the reaction with alkyl-substituted alkynyl carboxylic acids required CuI as a cocatalyst for high yield. The decarboxylation occurred even under high carbon monoxide pressure. The desired carbonylative coupling was formed from phenyl propiolic acid without any formation of a noncarbonylative coupling product in the absence of CuI. However, in the case of alkyl-substituted alkynyl carboxylic acids, CuI was required as a cocatalyst to ensure a high yield of the desired carbonylative product, as this was formed in low yield in the absence of CuI.

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발표분야: 유기화학

발표종류: 포스터, 발표일시: 금 15:00~17:00

## One-Pot Synthesis of Symmetrical and Unsymmetrical Aryl Sulfides by Pd-Catalyzed Couplings

박남진, 표아영, 이선우

전남대 화학과

This reaction method enables the one-pot synthesis of symmetrical and unsymmetrical diaryl sulfides by employing potassium thioacetate with aryl iodides and aryl bromides. The directed C-S bond formation from thioacetate has been discovered and successfully applied to the coupling of aryl bromides and a variety of thioacetates. In addition, this reaction condition was applied to the synthesis of symmetric and unsymmetric diaryl sulfide by use of thioacetate as a sulfur source. This method provided the tolerance to functional groups and foul smell-free environmental condition.

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발표코드: IV-ORGN.P-223

발표분야: 유기화학

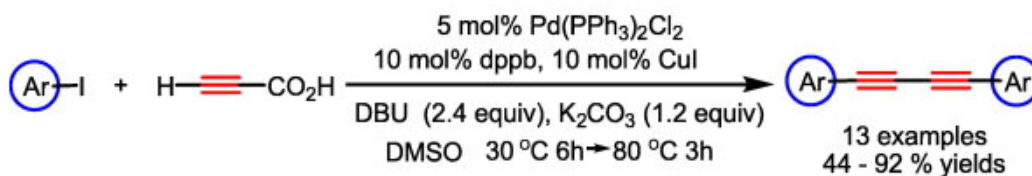
발표종류: 포스터, 발표일시: 금 15:00~17:00

## Synthesis of 1,4-Diarylsubstituted 1,3-Diynes from the SequentialCoupling Reactions of Propiolic Acid and Aryl Iodides

김용, 허유미, 이선우

전남대 화학과

1,4-Disubstituted 1,3-dialkynes were obtained from the one-pot palladium/copper-catalyzed coupling reactions of aryl iodide and propiolic acid. The optimized catalytic system consisted of 5.0 mol% Pd(PPh<sub>3</sub>)<sub>2</sub>Cl<sub>2</sub>, 10 mol% dppb, 10 mol% CuI, 2.4 equivalent of DBU and 1.2 equivalent of K<sub>2</sub>CO<sub>3</sub>. The coupling reaction was carried out at 30 °C for 6 h and subsequently at 80 °C for 3 h.



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발표분야: 유기화학

발표종류: 포스터, 발표일시: 금 15:00~17:00

## Synthesis of amido-N-imidazolium salts as ligands in Suzuki-Miyaura reactions : synthesis of milrinone and irbesartan.

manian rajesh kumar, 이선우

전남대 화학과

A new catalytic system based on palladium-amido-N-heterocyclic carbenes for Suzuki-Miyaura coupling reactions of heteroaryl bromides is described. A variety of sterically bulky, amido-N-imidazolium salts were synthesized in high yields from the corresponding anilines. Their catalytic system effectively promoted Suzuki-Miyaura couplings of heteroaryl bromides and chlorides with a range of boronic acids to give the corresponding aryl compounds in high yield. The yield was increased with increasing steric bulkiness of the substituted group. Especially, 1-(2,6-diisopropylphenyl)-3-N-(2,4,6-tri-tert-butylphenylacetamido)imidazolium bromide exhibited 850,000 TON in the coupling reaction of 2-bromopyridine and phenyl boronic acid. In addition, pharmaceutical compounds such as milrinone and irbesartan were synthesized via Suzuki-Miyaura coupling using sterically bulky, amido-N-imidazolium salt as a ligand.

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발표분야: 유기화학

발표종류: 포스터, 발표일시: 금 15:00~17:00

## Toward the total synthesis of Phorbaketal A

정시원, 이희윤

KAIST 화학과

Phorbaketal A was isolated by Rho et al. in 2009 from the Korean marine sponge *Phorbas sp.* and it exhibits cytotoxicity against human colorectal, hepatoma, and lung cancer cell lines. Phorbaketal A possesses an unprecedented structure that is novel spiro[5,5]ketal fused to a hydrobenzopyran ring. Its structure was elucidated by spectral and chemical methods. However, the absolute stereochemistry still has been in debates. We were attracted by its unique structure and started synthetic studies on Phorbaketal A in order to confirm the absolute stereochemistry of the natural product.

The key feature of current synthetic route is the Pd catalyzed terminal alkyne – internal alkyne coupling followed by Au and acid catalyzed cyclization of diol and internal alkyne. In addition to the confirmation of the structural identity of phorbaketal A, we expect that this synthetic strategy can be extended to the structural manipulation of Phorbaketal A for further biological study. Now we are investigating conditions for these key reactions.

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발표분야: 유기화학

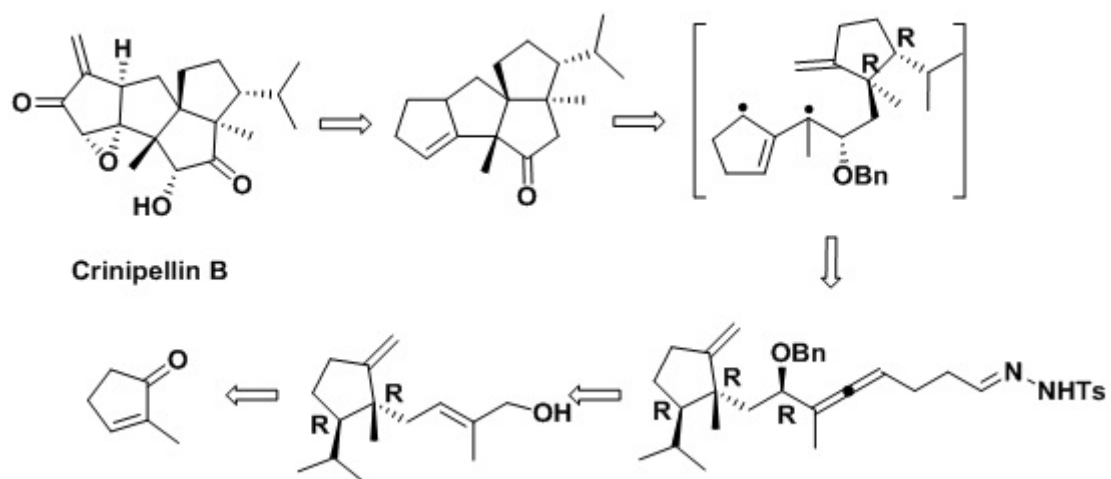
발표종류: 포스터, 발표일시: 금 15:00~17:00

## Total synthesis of (-)-Crinipellin B

강택, 이희윤

KAIST 화학과

Crinipellins are only one group of natural product having tetraquinane framework and isolated from the culture broth of the basidiomycete *Crinipellis stipitaria*. Crinipellins are active against gram-positive bacteria, yeasts, filamentous fungi, and Ehrlich carcinoma ascites cells. The structural uniqueness and biological activity make crinipellins attractive targets for synthesis. Crinipellin B is one of crinipellins and highly oxygenated substance contains eight stereogenic centers. Although there have been a lot of synthetic approaches to crinipellin B, because of its unprecedented structure, there has been only one report of the total synthesis of crinipellin B in racemic form. The intramolecular cycloaddition reaction of 1,3-trimethylenemethane(TMM) diyl was successfully utilized in construction of tetraquinane core structure and could be generated from allene and N-toluenesulfonylhydrazine. For asymmetric synthesis of crinipellin B, chiral resolution or induction methodology furnished highly enantiomerically pure chiral intermediate. Preparation of tetraquinane structure of crinipellin B with proper stereochemistry was succeeded through TMM diyl cycloaddition reaction, and further functional group modification furnished the formal total synthesis of crinipellin B.





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발표분야: 유기화학

발표종류: 포스터, 발표일시: 금 15:00~17:00

## **Ratiometric Detection of Mitochondrial Glutathione with a Two-Photon Probe**

**MASANTA GOUTAM**, \*임창수, \*\*김형중, \*조봉래, \*\*김환명

아주대 분자과학기술연구센터 \*고려대 화학과 \*\*아주대 에너지시스템학부

Glutathione is the most abundant cellular thiol, whose concentration ranges from 1 to 15 mM. Mitochondrial glutathione (mGSH) has great importance in maintaining cell viability and limiting damage to various potentially toxic treatments. Herein, we report a new TP probe that shows specifically targeting the mitochondria and ratiometric fluorescent change through reductive cleavage of its disulfide bond by glutathione. It can be excited by 750 nm femtosecond pulses and quantitatively detect mGSH in live cells and living tissues at a depth of >100  $\mu\text{m}$  without interference from other biologically relevant species by two-photon microscopy.

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발표분야: 유기화학

발표종류: 포스터, 발표일시: 금 15:00~17:00

## Hydrogenative Cyclization of allenynes including Theoretical calculation

윤효상, 김효동, \*강윤경, 장혜영

아주대 에너지시스템학부 \*서울대 화학과

Pt Complexes were modified with phosphine ligands,  $\text{SnCl}_2$  and  $\text{H}_2$  for the cyclization of allenynes, providing hetero- and carbocycle with completely controlled regio- and stereoselectivity. For the development of clean and cost-effective synthetic protocols, hydrogen is used as a reductant, and large amounts of toxic metallic compounds are avoided under our conditions. A possible catalytic cycle was proposed based on deuterium labeling study and theoretical calculation.

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발표코드: IV-ORGN.P-229

발표분야: 유기화학

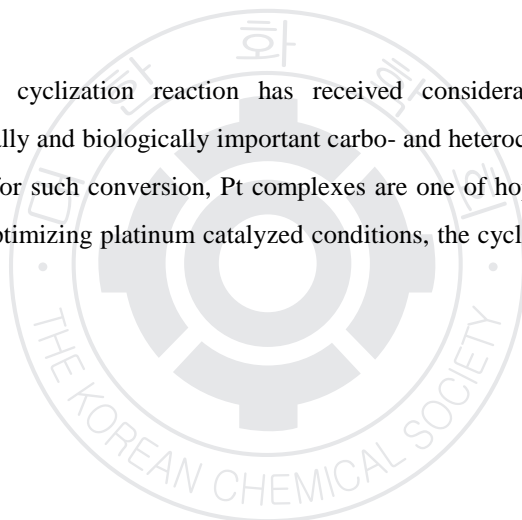
발표종류: 포스터, 발표일시: 금 15:00~17:00

## Platinum-catalyzed Michael Cyclization

김효동, 장혜영

아주대 에너지시스템학부

Transition metal-catalyzed cyclization reaction has received considerable attention due to their application to the synthetically and biologically important carbo- and heterocyclic building block. Among the metal complexes used for such conversion, Pt complexes are one of hopeful catalysts for hydrogen-mediated cyclization. By optimizing platinum catalyzed conditions, the cyclization of alkene-enones was accomplished.



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발표분야: 유기화학

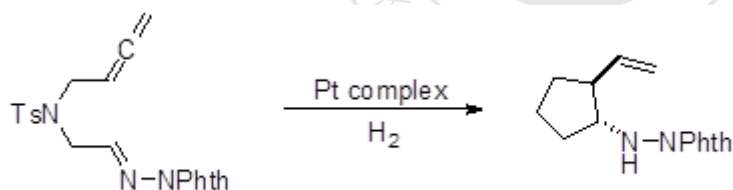
발표종류: 포스터, 발표일시: 금 15:00~17:00

## Platinum(II)- Catalyzed Cyclization of Allene-Hydrazones

김지환, 장혜영

아주대 에너지시스템학부

The allene-hydrazones were subjected to hydrogenation conditions, where allylplatinum complexes were generated from the allene, Pt catalysts, and H<sub>2</sub> without large amounts of organometallic reagents. Most allylmetal complexes exhibit the electrophilic property, rendering the reactions with nucleophiles. However, under our reaction conditions, charge reversed allylplatinum complexes are produced to react with the electrophile such as hydrazones. For the optimization of the reaction conditions, several phosphine ligands and additives are applied.



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발표코드: IV-ORGN.P-231

발표분야: 유기화학

발표종류: 포스터, 발표일시: 금 15:00~17:00

## Platinum(II)-catalyzed reductive cyclization of Allene-oximes

오현지, 장혜영

아주대 에너지시스템학부

The reductive cyclization of allene-oximes was studied under environmentally benign hydrogenation conditions. In addition to achiral oximes, the allene was added to chiral oximes. Various nitrogen-tethered allene-oximes efficiently undergo Pt-catalyzed reductive cyclization to afford five-membered rings. To generate catalysts,  $\text{PtCl}_2$ ,  $\text{SnCl}_2$ , phosphane and  $\text{H}_2$  were used. In this paper, we describe optimization results and the substrate scope of the environmentally friendly hydrogenative cyclization of allene-oximes.

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발표코드: IV-ORGN.P-232

발표분야: 유기화학

발표종류: 포스터, 발표일시: 금 15:00~17:00

## Platinum-catalyzed Hydrogenative Cyclization of 1,5-Bisallenes

임유나, 김효동, 윤효상

아주대 에너지시스템학부

The transition metal-catalyzed reaction of allenes has emerged as a useful protocol to prepare synthetically useful cyclic compounds. To carry out the cyclization using bisallenes, platinum catalysts were utilized in the presence of hydrogen. Remarkably, our catalytic system provided the desired cyclized product with high levels of regio- and diastereoselectivity. A tentative mechanism involving hydrometallation of the allene by the hydrido-platinum complex was proposed based on deuterium labeling studies and the stereochemistry of bisallene cyclization products.

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발표분야: 유기화학

발표종류: 포스터, 발표일시: 금 15:00~17:00

## Synthesis of a New Fluorescent Small Molecule Probe and Its Use for in vivo Lipid Imaging

이재홍, 김일향, \*이귀빈, \*\*배명애, \*\*\*안진희

고려대 화학과 \*서강대 화학과 \*\*한국화학연구원 신약플랫폼기술팀 \*\*\*한국화학연구원 대사성  
질환연구팀

A new small molecule probe for in vivo lipid imaging, LipidGreen, was developed. LipidGreen stained lipid droplets in 3T3L1 cell lines and fat deposits in zebrafish without apparent toxicity up to 100 uM. The utility of LipidGreen as a drug screening platform for fat regulation was also demonstrated in live zebrafish.

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발표분야: 유기화학

발표종류: 포스터, 발표일시: 금 15:00~17:00

## **Fabrication of various thicknesses based on self-assembly of block copolymer.**

이성우

홍익대 화학공학과

Block copolymers have been investigated for fabricating functional nanomaterials due to their properties of self-assembly. We prepared polystyrene-b-poly(2-vinyl pyridine) (PS-b-P2VP) lamellar films which is hydrophobic block-hydrophilic polyelectrolyte block polymer have 57 kg/mol-b-57 kg/mol. The lamellar stacks are obtained by exposing the spin coated film under chloroform. The P2VP blocks were then quaternized and crosslinked to various extents using 5wt% of iodomethane. This study shows that the total film thicknesses change the absorbance band by affecting the thickness of layers consisting of PS-b-P2VP photonic crystals.



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발표분야: 유기화학

발표종류: 포스터, 발표일시: 금 15:00~17:00

## Development of environment sensitive fluorescent probe selective to $\beta$ 2-AR

elena, \*강효진, \*\*정상전

한국생명공학연구원 나노바이오센터 \*과학기술연합대학원대 나노바이오공학 \*\*한국생명공학  
연구원 바이오테크놀로지연구단

G protein-coupled receptors (GPCRs) comprise the largest family of receptors – the specialized transmembrane proteins that sense specific agonists outside the cell to activate inside signal transduction pathways inducing cellular responses. GPCRs are involved in a wide variety of physiological processes and, thus, the drugs targeting members of this integral membrane protein family, which transmit chemical signals into a wide range of different cell types, represent the core of modern medicine. Among them,  $\beta$ 2-adrenergic receptor ( $\beta$ 2-AR) is a structurally characterized and well-studied prototype GPCR. Based on its three dimensional structure we designed and synthesized a specific probe by combination of  $\beta$ 2-adrenergic receptor specific ligand and environment sensitive fluorescent motif. The structure design of a novel fluorescent probe is derived from three well known synthetic moieties -propranolol ( $\beta$ 2-AR antagonist) as a specific ligand; polyethylene glycol chain as a modulator of molecular hydrophobicity and Badan as environment sensitive dye. The combination of these properties allows the bio-probe to be more fluorescent in hydrophobic media than in hydrophilic environment thereby becoming strongly fluorescent by specific binding to the hydrophobic pocket of  $\beta$ 2-AR in aqueous solution. This lead us to test the designed compound as environment sensitive fluorescent probe selective to  $\beta$ 2-AR.

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발표분야: 유기화학

발표종류: 포스터, 발표일시: 금 15:00~17:00

## Label-free fluorescent probe selective to HMG-CoA reductase.

김주환, \*강효진, \*\*정상전

과학기술연합대학원대 나노바이오공학과 \*과학기술연합대학원대 나노바이오공학 \*\*한국생명  
공학연구원 바이오테크놀로지연구단

Elevated cholesterol levels are a primary risk factor for coronary artery disease. Since 3-hydroxy-3-methyl glutaryl coenzyme A reductase (HMG-CoA reductase) catalyzes the rate-limiting step in the cholesterol biosynthetic pathway its selective inhibitors have been developed as powerful and safe therapeutics to lower cholesterol levels in plasma. Statins including simvastatin, lovastatin, rosuvastatin etc. represent such cholesterol lowering agents, which selectively bind to the substrate-binding site of HMG-CoA reductase. We have developed a new fluorescent detection technology for target proteins without target labeling, so called iFRET. In this study, we have prepared iFRET probes selective to HMG CoA reductase by combining a key structural motif of statin and a new iFRET acceptor motif. Since this fluorescence motif emits significant light at a longer wavelength close to 500 nm the probes may facilitate to image HMG CoA reductase even in cells as well as in vitro. The principle of iFRET and their use to detect HMG CoA reductase will be presented in this conference.

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발표분야: 유기화학

발표종류: 포스터, 발표일시: 금 15:00~17:00

## AM SURE<sup>TM</sup> resin: Novel Solution for Solid-phase Synthesis

김경민, \*김기선, 이윤식

서울대 화학생물공학부 \*비드테크 연구개발팀

AM PS (aminomethyl polystyrene) resin, which is a primitive solid support for solid-phase peptide synthesis (SPPS), has been widely used as a basic polymer material for the linker-loaded resins. In this research, we prepared AM SURE (aminomethyl surface-layered resin), characterized by its core-shell structure, in which aminomethyl groups are mainly located in the surface layer of the resin bead. This feature effectively solves the diffusion problem of reagents into the inner-part of the resin. First, phthalimidomethyl PS resin, the precursor to AM PS resin, was synthesized from 1% DVB-PS resin by using N-(chloromethyl)phthalimid. By removing the phthalimido groups, AM PS resin was obtained. Then, the core-shell structure was constructed by two simple steps; acetylation to AM PS resin using acetic anhydride, followed by partial hydrolysis of the acetyl group. The core-shell structure of AM SURE resin was confirmed by confocal laser scanning microscope (CLSM). But this method gave the aggregation problem of the resin. To overcome the problem we converted AM SURE to AM SURE HCl salt. In order to evaluate linker-loading kinetics, coupled to AM SURE. As expected, AM SURE showed better kinetic efficiency than non-core shell type one. In the following experiments, we synthesized various model peptides and proved that the resin gave good performance compared to the non-core shell type linker-loaded resin.

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발표분야: 유기화학

발표종류: 포스터, 발표일시: 금 15:00~17:00

## **Facile method for tunable magnetization for silica coated monodispersed sized superparamagnetic microsphere**

김경민, \*조상필, 이윤식

서울대 화학생물공학부 \*비드테크

Because the magnetic microsphere has several key advantages of quick, easy and gentle separation of biological compounds by using external magnetic field gradient, magnetic microspheres are widely used in biomedical field as a solid support for immunoassays, DNA sequencing and cell analysis. This paper presents a facile method for preparation of silica coated monodispersed superparamagnetic microsphere which tunable magnetic intensity. The core part of the magnetic bead was composed of magnetic nanoparticle(NP)-embedded sulfonated polystyrene bead. The outer part was surrounded with silica shell on which can provide water compatibility, easy modification and stability. The magnetic strength was controlled by loading level of sulfonation. The monodispersed magnetic beads were used as a substrate for protein separation. As a model application, streptavidin-bound magnetic beads were used to illustrate selective separation. The silica shell structure of magnetic bead was conformed by hysteresis analysis.

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장소: 제주ICC

발표코드: IV-ORGN.P-239

발표분야: 유기화학

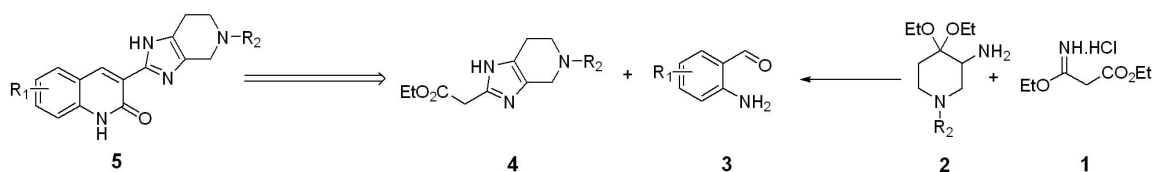
발표종류: 포스터, 발표일시: 금 15:00~17:00

## Efficient Synthesis of 2(4,5,6,7-Tetrahydro-1H-Imidazol[4,5-c]pyridin-2-yl)Acetate

양은혜

한국화학연구원 난치성질환치료제연구센터

Imidazoles frequently are found in biologically active natural products or pharmaceutically important drugs. Our interest in the search for new receptor tyrosine kinase inhibitors has been focusing on the synthesis of 2-quinolinone core derivatives **5** with C-3 imidazole moiety. The quinolin-2(1H)-one-3-imidazoles **5** were readily prepared by condensing of 2-imidazole-2-ylacetate **3** with variously substituted 2-aminobenzaldehydes **4**. In order to prepare 2-imidazole-2-ylacetates **3**, we chose to use Lawson's method for the synthesis of imidazoles by condensation of  $\alpha$ -aminoketals with imidates. Condensation of  $\alpha$ -aminoketals with imidates, followed by cyclization in refluxing 4M-HCl/Dioxane, yielded 2-imidazole-2-ylacetates under one-pot and mild reaction conditions.



일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: IV-ORGN.P-240

발표분야: 유기화학

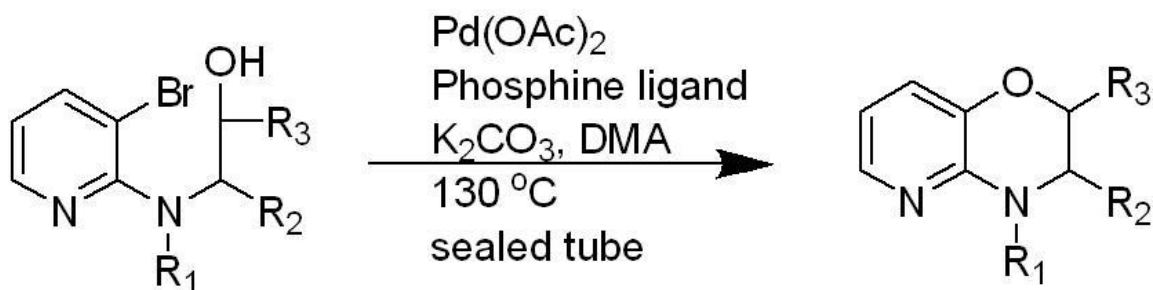
발표종류: 포스터, 발표일시: 금 15:00~17:00

## Synthesis of Pyrido[3,2-b][1,4]oxazines via Palladium-catalyzed Intramolecular Cyclization of Aminonoalcohol-tethered 3-bromopyridines

최지원

서강대 화학과

3,4-Dihydro-2H-pyrido[3,2-b][1,4]oxazines often display important biological activities. Although several methods for the synthesis of various 3,4-dihydro-2H-pyrido[3,2-b][1,4]oxazines have been described in the literature, those methods suffered in terms of low yields and were hard to give the optically pure compounds. Key intermediates, 2-(3-bromopyridine-2-ylamino)alcohols were obtained through a rapid nucleophilic substitution reaction of 3-bromo-2-chloropyridine with various aminoalcohols under microwave irradiation. With 2-(3-bromopyridine-2-ylamino)alcohols in our hands, palladium-catalyzed cyclization reaction of 3-bromoaminoalcohols cleanly afforded the pyrido[1,4]oxazine derivatives in 50-80% yield. Using this method, we can readily obtain optically pure 3,4-dihydro-2H-pyrido[3,2-b][1,4]oxazines with various substituents.



일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: IV-ORGN.P-241

발표분야: 유기화학

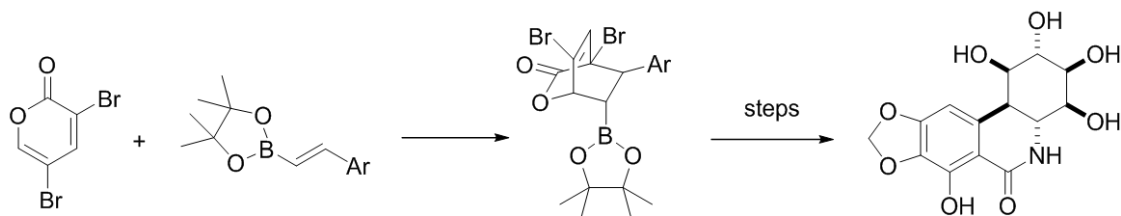
발표종류: 포스터, 발표일시: 금 15:00~17:00

## Vinylboronate as a synthetic equivalent of vinyl alcohol in the cycloaddition with 3,5-dibromo-2-pyrone en route to the total synthesis of ( $\pm$ )-pancratistatin

조현규, 조천규

한양대 화학과

Pancratistatin is a natural compound that was initially extracted from Spider Lily, a Hawaiian native plant that belongs to the family of Amaryllidaceae. It has been shown to have potent anti-cancer activities and selectively induce apoptosis in several human cancer cell lines. The promising biological activity and natural paucity has made pancratistatin an interesting target for total synthesis. Ever since the first total synthesis reported by Danishefsky and coworkers in 1989, many research groups around the world have presented novel strategies and routes to this natural compound. A few years ago, we have reported the first total synthesis of trans-dihydronarciclasine, very close congener of pancratistatin, by utilizing Diels-Alder reaction of 3,5-dibromo-2-pyrone. We have further envisioned the use of vinylboronate as dienophile would allow for the installation of the hydroxy group. Herein, we report the preliminary account of our new strategy toward the total synthesis of ( $\pm$ )-pancratistatin.



일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: IV-ORGN.P-242

발표분야: 유기화학

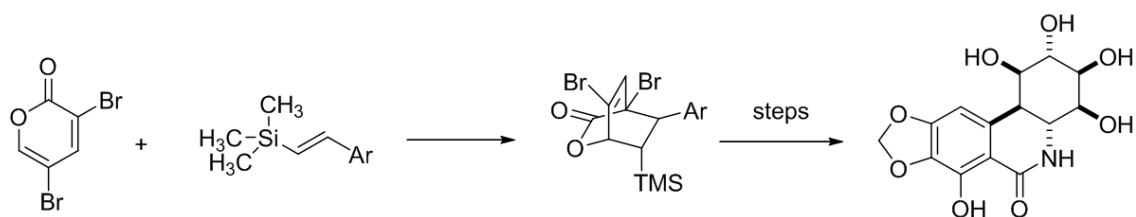
발표종류: 포스터, 발표일시: 금 15:00~17:00

## Use of vinylsilane in the cycloaddition with 3,5-dibromo-2-pyrone for the total synthesis of (±)-pancratistatin

정용근, 조천규

한양대 화학과

Pancratistatin is a natural compound that was initially extracted from Spider Lily a Hawaiian native plant that belongs to the family of Amaryllidaceae. It has been shown to have potent anti-cancer activities and selectively induce apoptosis in several human cancer cell lines. The promising biological activity and natural paucity has made pancratistatin an interesting target for total synthesis. Ever since the first total synthesis reported by Danishefsky and coworkers in 1989, many research groups around the world have presented novel strategies and routes to this natural compound. A few years ago, we have reported the first total synthesis of trans-dihydronarciclasine, very close congener of pancratistatin, by utilizing Diels-Alder reaction of 3,5-dibromo-2-pyrone. We have further envisioned the use of vinylsilane as dienophile would provide a handle for the easy installation of the hydroxy group. Herein, we report the preliminary account of our new strategy toward the total synthesis of (±)-pancratistatin.





일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: IV-ORGN.P-243

발표분야: 유기화학

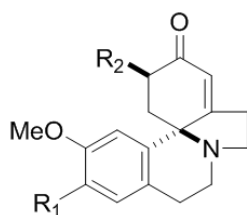
발표종류: 포스터, 발표일시: 금 15:00~17:00

## Studies toward the total syntheses of ( $\pm$ )-3-demethoxyerythratidinone, ( $\pm$ )-erysotramidine erythratinone and ( $\pm$ )-coccudinone

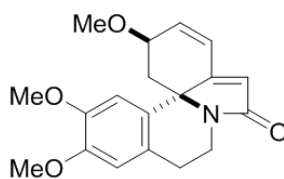
송지영, 조천규

한양대 화학과

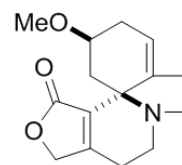
Widely distributed in the plant kingdom, the erythrina alkaloids are comprised of more than 70 natural products. Possessing an intriguing azatetracyclic framework in common, they represent attractive synthetic targets for their intriguing pharmacological effects that include sedative, hypotensive, neuromuscular blocking and CNS activity. For further extension of our 2-pyrone strategy toward the target-oriented synthesis, we set out the synthesis of ( $\pm$ )-3-demethoxyerythratidinone, ( $\pm$ )-erysotramidine and ( $\pm$ )-coccudinone. Herein, we report the preliminary account of the strategic use of our 2-pyrone Diels-Alder chemistry toward the total syntheses of the title alkaloids.



R<sub>1</sub>=OMe, R<sub>2</sub>=H: 3-demethoxyerythratidinone  
R<sub>1</sub>=H, R<sub>2</sub>=OMe: coccudinone



erysotramidine



cocculolidine

일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: IV-ORGN.P-244

발표분야: 유기화학

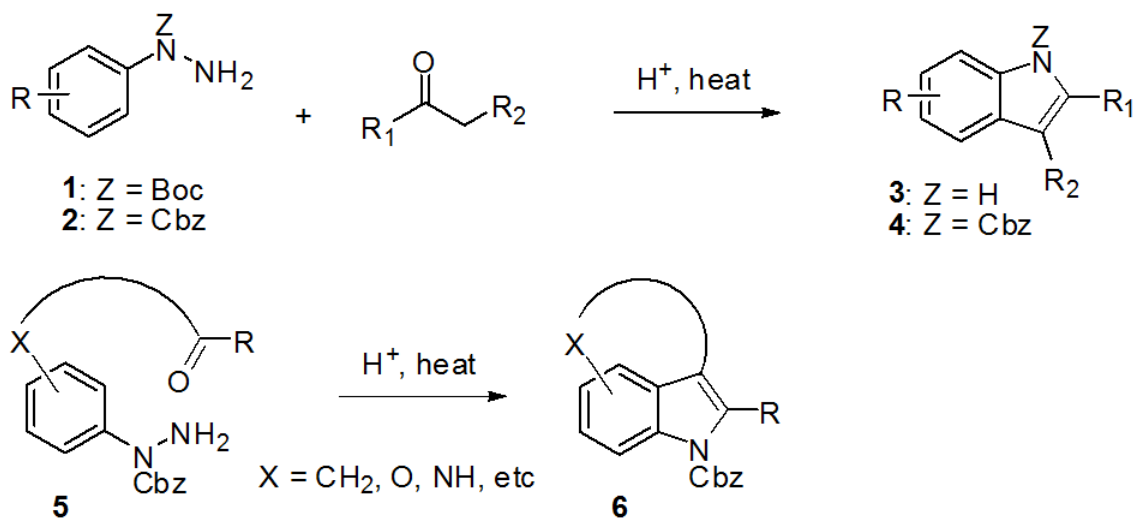
발표종류: 포스터, 발표일시: 금 15:00~17:00

## Intramolecular Fischer indolization reactions for the efficient construction of novel indolophanes

박인걸, 조천규

한양대 화학과

We have previously demonstrated that aryl hydrazides **1** 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 ( $1 \rightarrow 3$ ). 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 **2** can proceed in a Fischer indolization reaction to give *N*-Cbz-indole **4** 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 ( $5 \rightarrow 6$ ).



일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: IV-ORGN.P-245

발표분야: 유기화학

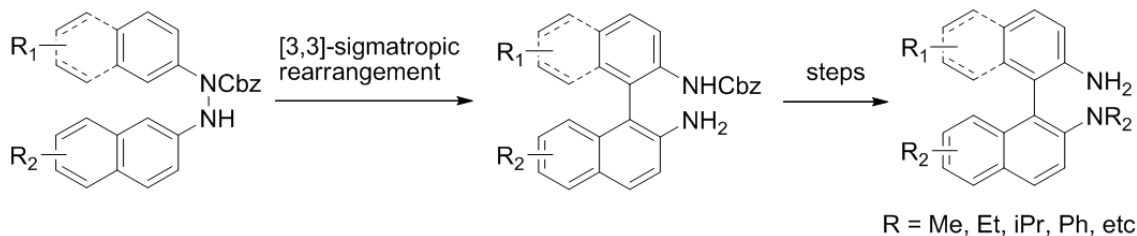
발표종류: 포스터, 발표일시: 금 15:00~17:00

## Facile generation of new non-symmetrically substituted 1,1'-binaphthyl-2,2'-diamines

임병윤, 서성은, 조천규

한양대 화학과

Axially chiral biaryls are important structural motifs as versatile auxiliaries for various asymmetric synthetic transformations. Their biaryl cores are primarily prepared through the Cu(II), Fe(III), Mn(III) or V(IV)/O<sub>2</sub> mediated oxidative couplings of aryl alcohols. The resultant 1,1'-biaryl-2,2'-diols then serve as platforms for the generation of other biaryl ligands including the famous 2,2'-bis(diphenylphosphino)-1,1'-binaphthyl (BINAP). While much less explored, the nitrogen analogues, 1,1'-binaphthyl-2,2'-diamine (BINAM) and its derivatives have recently gained much interest, not only as chiral ligands, but also as catalysts. However, further exploitation to their full potential is much hampered by the lack of general synthetic methods. Unlike the case with BINOL, the oxidative coupling reaction of aryl amines gives only limited success. Although an acid catalyzed rearrangement reaction of diaryl hydrazine may provide a quick solution, the poor accessibility to the starting diaryl hydrazines imposes severe limitation. We have previously reported that *N*-Cbz-diaryl hydrazides can undergo [3,3]-sigmatropic rearrangement reactions. The resultant mono-*N*-Cbz-1,1'-biaryl-2,2'-diamines can be readily manipulated into various other non-symmetrically substituted 1,1'-binaphthyl-2,2'-diamines.



일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: IV-ORGN.P-246

발표분야: 유기화학

발표종류: 포스터, 발표일시: 금 15:00~17:00

## **Facile synthesis, photophysical properties of sulfur containing 2,6-disubstituted BODIPY fluorescent probes.**

김태일, \*김영미

단국대 화학과 유기화학전공 \*단국대 화학과

Sulfur containing 2,6-disubstituted boron dipyrromethene (BODIPY) dyes have been efficiently synthesized from BODIPY with in-situ generated chlorodimethylsulfonium chloride via electrophilic substitution reaction. These new thio-based BODIPY dyes exhibited valuable photophysical properties such as a broad red emission band with unusually large Stokes shift, thus suggesting their potential platform for biosensing applications.

일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: IV-ORGN.P-247

발표분야: 유기화학

발표종류: 포스터, 발표일시: 금 15:00~17:00

## Synthesis and evaluation of urea , thiourea analogs and N -phenylbenzamide as tyrosinase inhibitors

최형, 한병희, 강성권

충남대 화학과

Skin hyperpigmentation can be dependent on either an increased number of melanocytes or activity of melanogenic enzymes, such as tyrosinase. N-Phenylthiourea (PTU) has long been known as a reference inhibitor against tyrosinase with an IC<sub>50</sub> value of 1.8  $\mu$ M. In the course of our work on the development of new whitening agents, a series of urea and thiourea analogs and N -phenylbenzamide were prepared and evaluated as a inhibitors of tyrosinase and melanin formation.

일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: IV-ORGN.P-248

발표분야: 유기화학

발표종류: 포스터, 발표일시: 금 15:00~17:00

## Regiochemical Pathway in the Ring Opening Reactions of 1-[( $\alpha$ )-Methylbenzyl]-2-Acylaziridine

육철민, 하현준, \*이원구

한국의국어대 화학과 \*서강대 화학과

Aziridine as a nitrogen-containing three membered ring is a synthetically versatile fragment to elaborate diverse nitrogen-containing cyclic and acyclic molecules via a key reaction of ring opening. It has been known the the reactivity is dependent to the substituent of nitrogen. The reaction of unactivated aziridine bearing 1-methylbenzyl and 2-acyl groups with oxygen nucleophiles with assistant to the electrophiles such as proton and  $\text{BF}_3\text{OEt}_2$  as Lewis acid yielded  $\alpha$ -amino compounds. This tells us that the regiochemical pathway of unactivated aziridine proceeded with concomitant breakage of bond between aziridine ring nitrogen and less substituted carbon, whose result was completely opposite to the same ring openings of 1-methyl-1-methylbenzyl-2-acylaziridium ions. This implied that the regiochemical pathway is determined not only by the substituent of aziridine but the characteristics of electrophile for the formation of aziridinium ion.

일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: IV-ORGN.P-249

발표분야: 유기화학

발표종류: 포스터, 발표일시: 금 15:00~17:00

## siRNA Delivery Systems Using Targeting Peptides

박정우

포항공과대 화학과

Small interfering RNA (siRNA) has been applied for gene therapy as the powerful tools. siRNA can recognize and silence complementary sequence of target mRNA in the cell as well as inhibit the target protein expression. Even though siRNA has great therapeutic potential, application of siRNA still has several problems such as a cytotoxicity, low cellular uptake, poor target specificity, weak nuclease resistance and endosomal escape barrier. To overcome the obstacles of siRNA therapy, I used two types of delivery systems. One is peptide-siRNA Conjugation method. In this method, Various peptides introduced to the siRNA using covalent bond such as a disulfide bond. The other is Peptide-siRNA complexation methods using charge-charge interaction between siRNA and peptide. Both systems show good cellular uptake and no cytotoxicity.

일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: IV-ORGN.P-250

발표분야: 유기화학

발표종류: 포스터, 발표일시: 금 15:00~17:00

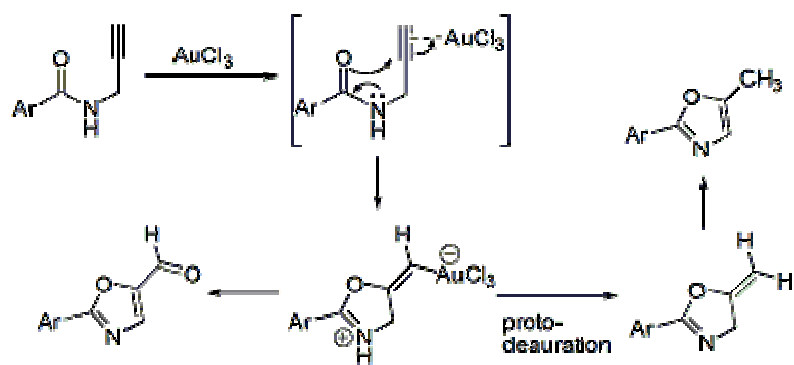
## Unusual Reaction Pathways of Vinylgold Complexes

서혜원

포항공과대 화학과

In last decade, gold catalyzed organic reactions have attracted great attention in organic and organometallic chemistry fields as efficient and new green chemistry tools. Especially gold catalyzed transformations of unsaturated carbon-carbon bonds have been extensively investigated, owing to the strong interactions between gold species and multiple bonds. Gold ions are soft acids owing to their strong s-orbital contraction/d-orbital expansion; they can strongly interact with multiple bonds which are soft bases.<sup>1</sup> Though numerous papers have reported efficient transformations through gold catalyzed activations of multiple bonds, only a handful of gold intermediates are characterized.<sup>2</sup> During our study on rhodamine-based fluorescent probes for gold species,<sup>3</sup> we observed unusual reaction products from the vinylgold intermediates. We observed formyl products rather than the protodeauration products expected (Scheme 1). This unexpected result drew our attention on the chemistry of vinylgold intermediates involved as well as on the mechanism of the formyloxazole formation. We have investigated the gold mediated cyclization for model substrates, N-(propargyl)benzamide and its derivatives, and details of which will be presented. Reference1. Gorin, D. J.; Toste, F. D.; Nature 2007, 446, 395.2. A. S. K. Hashmi, Angew. Chem. Int. Ed. 2010, 49, 5232.3. O. A. Egorova, H. Seo, A. Chatterjee, K. H. Ahn, Org. Lett. 2010, 12, 401.





Scheme 1. Formation of formyloxazoles and protodeauration products in a gold mediated cyclization.



일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: IV-ORGN.P-251

발표분야: 유기화학

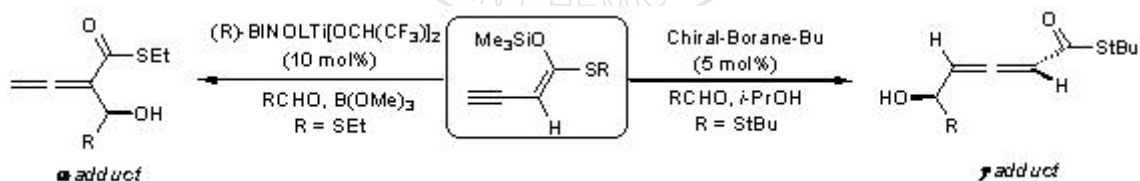
발표종류: 포스터, 발표일시: 금 15:00~17:00

## Catalytic Asymmetric Aldol Reactions of (S,O)-Keteneacetals with Aldehydes: $\alpha$ vs $\gamma$ Addition

김보미, 김지현, 유찬모

성균관대 화학과

Asymmetric aldol reactions have been regarded as one of the most efficient methods to construct chiral pools. Recently, we have developed a new method of the allenolate adol process in forming 2-hydroxy allenolate in high levels of enantioselectivity. In light of this result, we turned our attention to design catalytic versions of this approach. We would like to present herein several crucial points including stereochemical pathways and absolute and relative stereochemistry that have emerged from our recent investigations: 1) reaction conditions for the  $\alpha$  vs  $\gamma$  Addition adducts 2) Synthesis of natural lignan copounds.



일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: IV-ORGN.P-252

발표분야: 유기화학

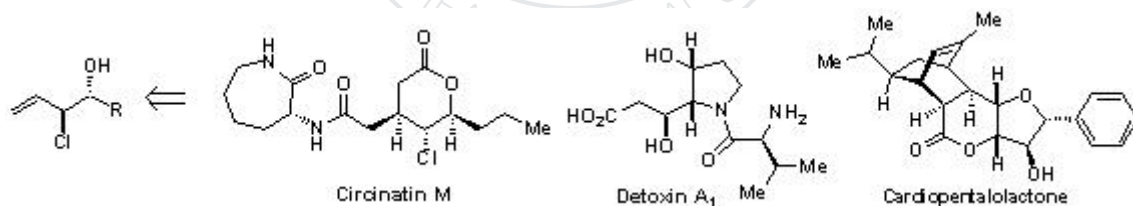
발표종류: 포스터, 발표일시: 금 15:00~17:00

## Application of Asymmetric Chloroallylboration for the Synthesis of Natural Products

최지훈, 양보나, 유찬모

성균관대 화학과

In light of widespread advances in synthetic methods for the synthesis of chiral substances, the allylic transfer reactions of carbonyl functionalities using chiral auxiliaries or catalysts led to significant developments in the area of asymmetric synthesis. Recently, we have developed a new chloroallylboration for the synthesis of enantiomerically enriched chlorohydrins and vinyl oxiranes. We would like to present herein several synthetic applications for the synthesis of naturally occurring detoxin and cardiopentalolactone.



일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: IV-ORGN.P-253

발표분야: 유기화학

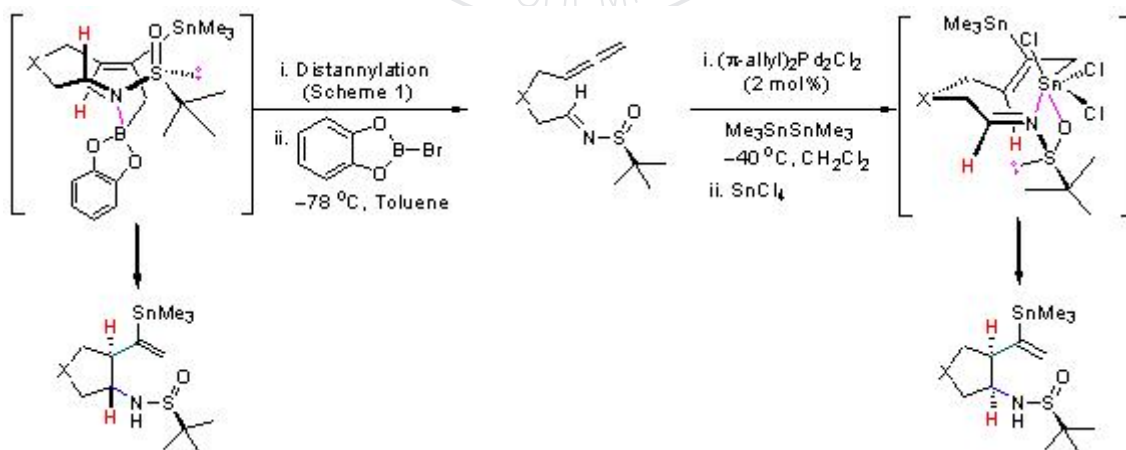
발표종류: 포스터, 발표일시: 금 15:00~17:00

## Control Factors for Diastereoselectivity in the Cyclization of Allenyl Sulfinimide through an Intramolecular Allylic Addition

곽진호, 최지훈, 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. Recently, we disclosed our discoveries of the cyclization methods for the synthesis of cyclic compounds from allenyl carbonyls and allenyl hydrazones by using transition metals, as parts of the allylic transfer strategy using allenes as asubstrates or intermediates. We wish to present our discovery of a remarkable additive and solvent effect as introduction of the sulfinimide for the conversion of cis or trans adducts.



일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: IV-ORGN.P-254

발표분야: 유기화학

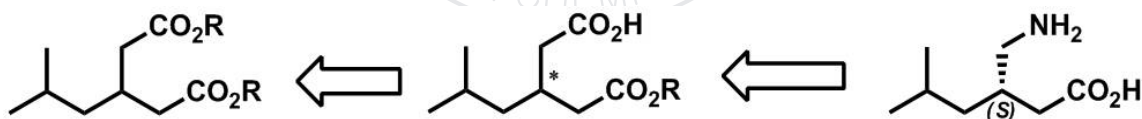
발표종류: 포스터, 발표일시: 금 15:00~17:00

## Lipase Mediated Desymmetrization of 3-isobutyl-1,5-pentanedioates: Asymmetric synthesis of Pregabalin

윤두하, 하현준, \*이원구

한국의국어대 화학과 \*서강대 화학과

(S)-(+)-3-aminomethyl-5-methylhexanoic acid known as Pregabalin is a lipophilic GABA ( $\gamma$ -aminobutyric acid) analogue for the treatment of several central nervous system disorders including epilepsy, neuropathic pain, anxiety and social phobia. Successful preparation of pregabalin was achieved from CALB catalyzed desymmetrization of prochiral dialkyl 3-isobutyl-1,5-pentanedioate to yield 3-((alkyloxycarbonyl)methyl)-5-methylhexanoic acid in high yield with high optical purity. The ester part of the hydrolytic product was converted to amide followed by Hoffman rearrangement to yield the product in overall 52% yield.



일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: IV-ORGN.P-255

발표분야: 유기화학

발표종류: 포스터, 발표일시: 금 15:00~17:00

## Comparison of butylcholinesterase inhibition activity between two linkers used for (R)-Lipoic acid-polyphenol hybridization

연고훈, \*이슬기, \*한준석, \*이현진, \*\*임용배, \*\*\*김현주, \*\*\*\*이봉호, \*\*\*\*박정호

한밭대 응용화학과 \*한밭대 생명공학과 \*\*한밭대 응용화학 \*\*\*한밭대 응용화학 생명공학과  
\*\*\*\*한밭대 응용화학생명공학부

Alzheimer's disease is an irreversible, progressive brain disease that reduces the amount of neurotransmitter, acetylcholine (ACh), existing in the patient's brain and slowly destroys memory and thinking skills. Cholinergic drugs developed to treat AD are inhibitor for acetylcholinesterase (AChE). Since growing evidence that butyrylcholinesterase (BuChE) also contributes to ACh regulation and function in cholinergic transmission, we have carried out research to find out the selective inhibitor for BuChE. On this poster we present the comparison of butylcholinesterase inhibition activity between two linkers [2-(2-aminoethoxy)-ethanol and 1-(2-hydroxyethyl)-piperazine] used for (R)-Lipoic acid-polyphenol hybridization. 1-(2-Hydroxyethyl)-piperazine linker showed better inhibition effect for BuChE than 2-(2-aminoethoxy)-ethanol linker.

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발표분야: 유기화학

발표종류: 포스터, 발표일시: 금 15:00~17:00

## The [4+2] Dipolar Cycloaddition between Propiolic Acid and Alkenes through Gold Catalysis: Synthesis of $\alpha,\beta$ -Unsaturated- $\delta$ -Lactones

염현석, 신승훈

한양대 화학과

The  $\alpha,\beta$ -unsaturated- $\delta$ -lactone moiety is present in a number of bioactive natural products such as massoialactone, goniotalamin, and fostriecin, having a wide range of biological activities. Also, commercially available drugs such as Lipitor (Pfizer), Zocor (Merck) have related lactone moiety. Therefore the development of efficient and concise synthetic method for this common structural motif will make significantly contribution to the chemistry related fields including chemical biology and medicinal chemistry. Traditionally, representative synthetic procedures for  $\alpha,\beta$ -unsaturated- $\delta$ -lactone include i) asymmetric allylation-RCM sequence, ii) asymmetric hetero DA-hydrolysis-oxidation sequence, and iii) diastereoselective ketene cycloaddition-ring expansion approach. These previously reported reactions suffer from limitations of multistep synthesis, which could often result in undesirable problems such as chemical compatibility issues and necessity of protecting groups, among others. Alkenes are easily available and have good functional group compatibility in a multi-step setting. Herein, we disclose preliminary results our study on the gold-catalyzed formal [4+2] dipolar cycloaddition between propiolic acid and alkenes for efficient assembly of  $\alpha,\beta$ -unsaturated- $\delta$ -lactones. A number of alkenes and allenes participate smoothly in this transformation with moderate to good isolated yields of the product lactone. This one-pot, redox-neutral approach could allow an easy and obvious disconnection in a retrosynthetic sense to various natural products having this core.

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발표분야: 유기화학

발표종류: 포스터, 발표일시: 금 15:00~17:00

## Efficient one-pot reaction of phosphoramiate (or phosphinamide) with 2,5-dimethoxytetrahydrofuran and 1,3-acetonedicarboxylic acid

정대일, 정수경, 이수지, 이언진, 송주현, \*한정태

동아대 화학과 \*영동대 뷰티케어과

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 pentylenetetrazol-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 nitrogen containing heterocycles, we now report a convenient one-pot synthesis of tropane compounds and nitrogen containing heterocycles in the reaction of phosphinamide (or phosphoramiate) with 2,5-dimethoxytetrahydrofuran, and 1,3-acetonedicarboxylic acid at 0°C (or reflux). And in order to obtain bioactive new compounds, we tried reaction of phosphinamide (or phosphoramiate), 2,5-dimethoxytetrahydrofuran, and 1,3-acetonedicarboxylic acid with dimethylacetylenedicarboxylate (or dienophiles).



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발표분야: 유기화학

발표종류: 포스터, 발표일시: 금 15:00~17:00

## **Benzyne Chemistry with amine, 2,5-dimethoxy tetrahydrofuran, and acetonedicarboxylic acid**

최순규, 장가영, 이상곤, 이도훈, 정대일, \*한정태

동아대 화학과 \*영동대 뷰티케어과

Aryl subunits are commonly found in a variety of biologically active and natural compounds, agrochemicals, HIV-1 protease inhibitors, and compounds of interest in material science. An efficient transition-metal free procedure for the N-arylation of amines has been achieved by allowing these substrates to react with a variety of O-silylaryl triflates in the presence of CsF. And also benzyne chemistry with amines, 2,5-dimethoxytetrahydrofuran, and 1,3-acetonedicarboxylic acid in acid solution has been done.

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발표분야: 유기화학

발표종류: 포스터, 발표일시: 금 15:00~17:00

## A Study on the Synthesis and reaction of 1,5,3,7-Diazaphosphocines

이용균, 이은수, 김윤영, 정대일, \*한정태

동아대 화학과 \*영동대 뷰티케어과

Great efforts have been devoted to the development of efficient ligands for transition metal, in order to obtain complexes whose stability, physical properties, and biodistribution could make them suitable for application as contrast agents for magnetic resonance imaging (MRI), diagnostic-therapeutic radiopharmaceuticals, or fluorescent bioassays. We now report reaction of the amino acids (or amines) with hypophosphorous acid and formaldehyde. And also cycloaddition of 1,5,3,7-diazadiphosphocine derivatives and Dimethyl acetylenedicarboxylate(or dienophiles) has been done.

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발표종류: 포스터, 발표일시: 금 15:00~17:00

## Synthesis of Biphenyl-diketones with Carbon Monoxide and Metal Carbonyl

이수지, 이상곤, 정대일, \*한정태

동아대 화학과 \*영동대 뷰티케어과

Terphenyl derivatives have been known to exhibit a variety of optical and electrical properties. Naturally isolated p-terphenyl metabolites are known to possess the potent biological activities. In our ongoing studies endeavored toward Wittig reaction of diketone formed by Suzuki carbonylative reaction with aryl ylide to afford stilbene derivative. We tried the reaction for 4,4'-diiodobiphenyl and arylboronic acid with carbon monoxide (or metalcarbonyl) via Pd(NHC) complex. Synthesized diketone products are biphenyl-4,4'-diylbis(phenylmethanone) and biphenyl-4,4'-diylbis(naphthalen-1-ylmethanone) and biphenyl-4,4'-diylbis(biphenyl-3-ylmethanone) and biphenyl-4,4'-diylbis(pyridin-4-ylmethanone).

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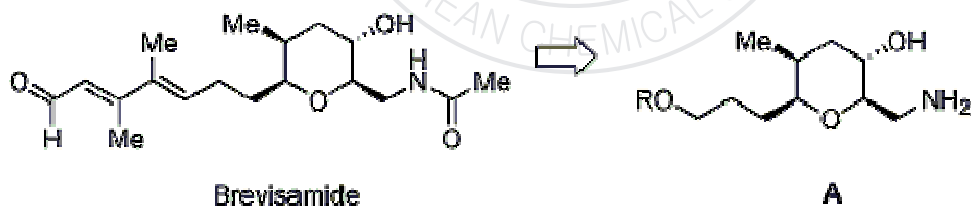
발표종류: 포스터, 발표일시: 금 15:00~17:00

## Synthetic study toward Brevisamide

강한영, 이정미

충북대 화학과

The brevitoxins, cyclic ethers which are responsible for massive death of fishes and marine animals, are produced by red tide dinoflagellate *Karenia brevis*. Brevenals are also produced from the same dinoflagellate, which is a smaller polyether and is an antagonist of brevitoxins. Another compound, brevisamide is also isolated as well, which can be regarded as a truncated analog of brevenal. There have been several reports on the synthesis of brevisamide. We have been interested in the total synthesis of brevisamide. Brevisamide could be synthesized from the acid A, which was used in the total synthesis reported previously. Our effort to synthesize this intermediate A will be presented.



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발표종류: 포스터, 발표일시: 금 15:00~17:00

## Rh(NHC)-Catalyzed *O*-Arylation of Aryl Bromides

김현진, \*장석복, \*\*김민

KAIST \*KAIST 화학과 \*\*University of California, San Diego

The first example of a rhodium-catalyzed *O*-arylation reaction of aryl bromides is reported. While a right combination of rhodium species and N-heterocyclic carbene (NHC) offered an effective catalytic system enabling the arylation under optimized conditions, the choice of NHC turned out to be most important for obtaining high catalytic activity. The developed *O*-arylation protocol is featured to have a wide range of substrate scope, a high level of functional group tolerance, and a novel flexibility allowing complementary routes to either N- or *O*-arylation depending on the type of NHC under otherwise similar Rh catalysis.

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발표종류: 포스터, 발표일시: 금 15:00~17:00

## Phosphorescent Dimesitylboryl-appended Iridium (III) Complex for F<sup>-</sup> Sensing

LIYINAN, 현명호

부산대 화학과

A novel outstanding fluoride ion-sensing phosphorescent iridium (III) complex bearing boryl group was prepared and its anion selective phosphorescent chemosensing behaviour was investigated. The new iridium (III) complex exhibits notable phosphorescence quenching for F<sup>-</sup> in acetonitrile solution with respect to the detection of other anions such as Cl<sup>-</sup>, Br<sup>-</sup>, I<sup>-</sup>, H<sub>2</sub>SO<sub>4</sub><sup>-</sup>, CN<sup>-</sup>, and NO<sub>3</sub><sup>-</sup>. The association constant for F<sup>-</sup> was calculated to 2.50 x 10<sup>4</sup> M<sup>-1</sup> according to the Benesi-Hildebrand expression. The new iridium (III) complex was proposed to utilized for the detection of F<sup>-</sup>.

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발표종류: 포스터, 발표일시: 금 15:00~17:00

## Stereoselective [5+2] oxidopyrylium ion cycloaddition reactions for the total synthesis of frondosins

권국태, 이희윤

KAIST 화학과

3-Oxidopyrylium ions can be regarded as  $4\pi$ -electron component for addition across the C-2 and C-6 position, and as  $6\pi$ -electron component for reaction across the C-2 and C-4 position. Therefore several groups have utilized 3-oxidopyrylium ion as a  $4\pi$ -electron component or a  $6\pi$ -electron component for the cycloaddition reaction. [5+2] Cycloaddition reaction of oxidopyrylium ion has been investigated, but in case of intramolecular version, there was a few examples.

Intramolecular cycloaddition of oxidopyrylium ion is a powerful tool for constructing bicyclic ring system containing 7-membered ring. And stereoselectivity of Intramolecular [5+2] cycloaddition reaction of oxidopyrylium ion and olefin can be controlled by substituents of olefin. Using this method, Frondosin A which has a 7,6 bicyclic ring system could be synthesized.

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발표종류: 포스터, 발표일시: 금 15:00~17:00

## Enantioselective synthesis of $\beta$ -(3-indolyl)-substituted carboxylates via Friedel-Crafts alkylation of indoles

강영구, 김대영

순천향대 화학과

The Friedel-Crafts (FC) reaction is one of the most powerful C-C bond-forming processes in organic chemistry. Indole derivatives are present in many substances commonly found in nature, as well as in many compounds that show pharmacological and biological activities. Simple alkenyl esters have proven to be difficult substrates for effective chirality relay in asymmetric catalysis because of essentially low reactivity of  $\alpha,\beta$ -unsaturated esters as Michael acceptors.  $\alpha$ -Keto phosphonates, which have the ability of the phosphorus to function as a leaving group, were introduced as activated ester surrogates. Herein, we wish to describe the enantioselective FC reaction of indoles with  $\delta,\gamma$ -unsaturated  $\alpha$ -keto phosphonates catalyzed by air- and moisture-stable chiral palladium complexes. The intermediate  $\gamma$ -indolyl  $\alpha$ -keto phosphonates easily were converted desired methyl esters and the alkylated products were obtained in good yields with excellent enantioselectivities (up to 99% ee).



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발표종류: 포스터, 발표일시: 금 15:00~17:00

## **Enantioselective synthesis of oxindoles bearing a quaternary stereocenter at the C3-position using bifunctional organocatalysts**

이현주, 김대영

순천향대 화학과

Oxindole structures exist in a large number of natural product and bioactive molecules. In particular, oxindole derivatives bearing a C3-quaternary carbon stereocenter are a versatile structural motif found in a variety of biologically and pharmaceutically active natural products and utilized as building blocks for indole alkaloid synthesis. In this presentation, we wish to describe the direct enantioselective Michael reaction of 3-substituted oxindoles with vinyl sulfone catalyzed by bifunctional organocatalysts. 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).

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발표종류: 포스터, 발표일시: 금 15:00~17:00

## Asymmetric aldol reaction of $\alpha$ -keto phosphonates: synthesis of chiral tertiary $\alpha$ -hydroxy phosphonates

이현주, 김대영

순천향대 화학과

$\alpha$ -Hydroxy alkylphosphonates have received attention both as substrates for the preparation of other  $\alpha$ -substituted phosphonates, and because of their inhibitory activity towards several important groups of enzymes and various classes of protein tyrosine kinases and phosphatases. In this presentation, we wish to report the enantioselective synthesis of  $\alpha$ -hydroxy alkylphosphates catalyzed by bifunctional organocatalysts. The corresponding tertiary  $\alpha$ -hydroxy alkylphosphonates were generally obtained in good yields with high enantioselectivities.

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발표분야: 유기화학

발표종류: 포스터, 발표일시: 금 15:00~17:00

## Chiral palladium (II) complexes catalyzed Mannich reaction of $\alpha$ -fluorinated $\beta$ -ketoesters with N-Boc aldimines

강영구, 김대영

순천향대 화학과

Chiral organofluorine compounds are interesting and important materials with uses in analytical, biological, and medicinal chemistry and also in the chemistry of polymers and materials. The Mannich reaction is a fundamental C-C bond-forming reaction in synthetic organic chemistry. Catalytic enantioselective Mannich reactions provide one of the most versatile and attractive approaches for the generation of optically active chiral amino acid derivatives. Among various strategies, electrophilic fluorination of active methines and C-C bond-formation reaction of fluorocarbon nucleophiles are two typical approaches for the construction of fluorine-containing molecules, and their asymmetric versions are particularly attractive. Enantioselective electrophilic fluorination has been achieved with the aid of electrophilic fluorinating agents. On the other hand, the use of fluorinated active methine nucleophiles for a catalytic asymmetric reaction has become increasingly popular. In this presentation, we wish to communicate herein Mannich reaction of  $\alpha$ -fluoro  $\beta$ -ketoesters using chiral palladium complexes. The Mannich reaction of  $\alpha$ -fluoro- $\beta$ -ketoester with N-Boc imines to give the corresponding Mannich adducts in good yields and stereoselective (up to 99% ee) for various of substrates.

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발표종류: 포스터, 발표일시: 금 15:00~17:00

## **Organocatalytic C-H bond functionalization via 1,5-hydride transfer and cyclization under microwave irradiation**

권유경, 강영구, 김대영

순천향대 화학과

Tetrahydroquinoline derivatives have attracted considerable attention from organic and medicinal chemists primarily because they display a wide range of physiological activities. Traditional methodologies for the formation of tetrahydroquinoline derivatives mainly include the Povarov reaction and reduction of quinolines. Recently, we have report the synthesis of tetrahydroquinolines through organocatalytic C-H bond functionalization via tandem 1,5-hydride transfer and ring closure. Despite significant advances in this field, one of the critical shortcomings of many organocatalysis reactions reported to date include long reaction times. In this presentation, we wish to communicate organocatalyzed C-H bond functionalization via microwave irradiation. This synthetic method afforded high yields of tetrahydroquinoline derivatives with remarkably short reaction time than thermal experimental conditions.

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## Studies on the synthesis of $\alpha$ -Azidoether as a reversible terminator for DNA SBS (sequencing by synthesis)

권태희, \*이재균, \*\*배애님, 이재열, \*\*조용서, \*\*민선준

경희대 화학과 \*KIST 케모인포매틱스연구단 \*\*KIST 생체과학연구본부

Over the past decades, DNA sequencing technology has become essential for various applied researches such as genomics, biotechnology, and biological systematics in addition to basic science area. Since the Sanger sequencing method dominated the industry, many next generation sequencing (NGS) methods have been developed for sequencing a large number of genomes with high efficiency and low cost. Recently, DNA sequencing by synthesis (SBS) approaches have been widely explored. The key feature of this method is that modified nucleotides attached to cleavable fluorophore moiety are required for repeating sequencing cycle. Herein, we report design and synthesis of new modified nucleotides having the reversible terminator at the 3'-OH position, which plays a dual role as a fluorescent signal reporter as well as a protective group. We are expecting that these new nucleotides replaced by  $\alpha$ -azidoether at the 3'-OH are effectively introduced to DNA polymerase during polymerization. In addition, the fluorophore on the DNA extension products after determination of base will be easily removed under a mild reaction condition which is compatible with DNA.

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발표분야: 유기화학

발표종류: 포스터, 발표일시: 금 15:00~17:00

## Studies on Intramolecular Aza-Prins-type Cyclization of Amino Allylsilane

손영욱, \*이재균, \*\*배애님, 이재열, \*\*민선준, \*\*조용서

경희대 화학과 \*KIST 케모인포매틱스연구단 \*\*KIST 생체과학연구본부

The tricyclic benzo[a]quinolizine ring system has been known as a constituent of biologically active natural products and pharmacological molecules. For example, it exists in a type of alkaloids such as berberine, emetine, and tetrabenazine (TBZ), which are known as potential drug candidates for neurological disorders. Although various methods for the construction of these classes of heterocycles are reported, the development of new efficient methods to synthesize such compounds are still challenging to the synthetic organic communities due to their structural novelty and application. Prins cyclization reaction is one of the useful synthetic strategies to construct five- or six- membered ring system containing oxygen or nitrogen heteroatom. In general, this reaction involves the electrophilic addition of alkenes or alkynes to oxonium or iminium intermediates generated from acid-catalyzed condensation of alcohols or amines with carbonyl compounds. Depending on appropriate control of the termination step, feasible functional groups would be introduced to the final cyclized products. In this study, we report an efficient synthesis of benzo[a]quinolizine moiety via aza-Prins-type cyclization of amino allylsilane. Unlike the conventional Prins-type reactions, we found that oxidative C-H activation of isoquinolines by DDQ or PIDA (phenyl iododiacetate) could successfully generate the corresponding iminium species, which underwent cyclization to afford the tricyclic benzoquinoline derivatives in good yields.

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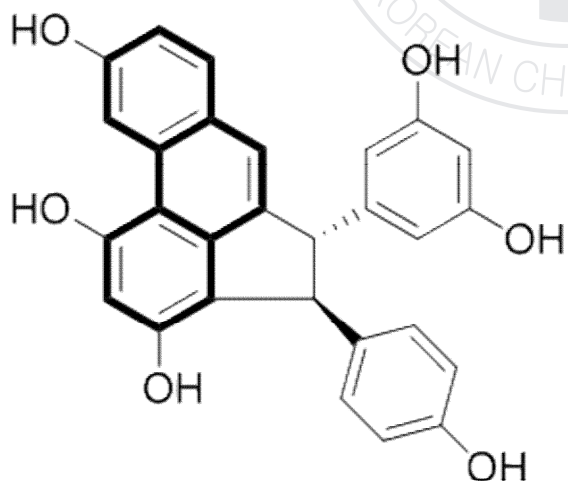
발표종류: 포스터, 발표일시: 금 15:00~17:00

## Total Synthesis of Laetevirenol A via Suzuki-Miyaura Coupling/Aldol Condensation Cascade Reaction

최영록, \*김성훈, \*\*허정녕

고려대 화학과 \*경북대 화학과 \*\*한국화학연구원 의약화학연구센터

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 the direct one-pot synthesis of a phenanthrene scaffold by employing a Suzuki-Miyaura coupling/aldol condensation cascade sequence, which can be further applied toward the total synthesis of Laetevirenol A



Laetevirenol A

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발표종류: 포스터, 발표일시: 금 15:00~17:00

## Direct conversion of esters to morpholine amides using diisobutyl(morpholino)aluminum

전아람, 서보람, 안덕근

강원대 화학과

The morpholine amides that a cheap and good substitute for Weinreb amides are valuable building blocks and useful intermediates for the synthesis of complex natural products with significant biological activity and other useful materials. A large number of synthetic methods to make morpholine amides from various have previously been reported. Among these, an aminolysis of acid chlorides are generally considered to be the method of choice. On the other hand, the direct synthesis of morpholine amides from esters recently reported only one method that using DABAL-Me<sub>3</sub> at 130 °C under microwave heating. Now, we have found that a useful direct conversion method of esters to morpholine amides using diisobutyl(morpholino)aluminum under mild reaction condition in excellent yields (81-99%).



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발표종류: 포스터, 발표일시: 금 15:00~17:00

## Efficient synthetic method of amides from acid chlorides using diisobutyl(amino)aluminum

박재교, 신원규, 안덕근

강원대 화학과

A useful and effective functional group transformation of various organic compounds is important in organic synthesis of natural products and materials with interesting properties. Amides in the organic compounds is one of important functional group and building block to make the valuable compound. Recently, we have found that a useful and new one-pot synthetic method of various amide including morpholine amide from common acid chlorides using diisobutyl(amine)aluminum for 10min in good yields (

일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: IV-ORGN.P-275

발표분야: 유기화학

발표종류: 포스터, 발표일시: 금 15:00~17:00

## A simple and effective partial reduction of acid chlorides to aldehydes

김소영, 이민지, 안덕근

강원대 화학과

The establishment of simple and effective partial reduction of acid chlorides to aldehydes is one of the most important and highly desired objectives in organic synthesis. And a large number of improved methods and reducing agents for this purpose have been reported. Also, we have reported that a new synthetic method using morpholine-PDBBA system showed effective partial reducing characteristics for various acid chlorides. However, we want to find more simple and effective methodology than reported methods to now for partial reduction of acid chlorides without preparing any reducing agents. Recently, we carried out experiences to find a simple and effective method under our purpose, as a results, we have found the new synthetic method of aldehydes from acid chlorides for short reaction time in almost quantitative yields using commercial available reagents only.

일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: IV-ORGN.P-276

발표분야: 유기화학

발표종류: 포스터, 발표일시: 금 15:00~17:00

## Quantitative synthetic method of aldehydes from nitriles

이민지, 김소영, 안덕근

강원대 화학과

The establishment of a simple, general and practical partial reduction of carboxylic acid derivatives to aldehydes is valuable tools in organic synthesis. Recently, we reported the results of partial reduction of nitriles using new class of reducing agents. However, the new partial reduction method using new reducing agents has a problem that could not be reacted aliphatic nitriles by new reducing agents. Therefore, we tried to find a new and simple method to solve problem of reported method successfully. Fortunately, we found the efficient synthetic methodology of aldehydes from both aromatic and aliphatic nitriles in quantitative yields using morpholine-DIBALH mixture system.

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장소: 제주ICC

발표코드: IV-ORGN.P-277

발표분야: 유기화학

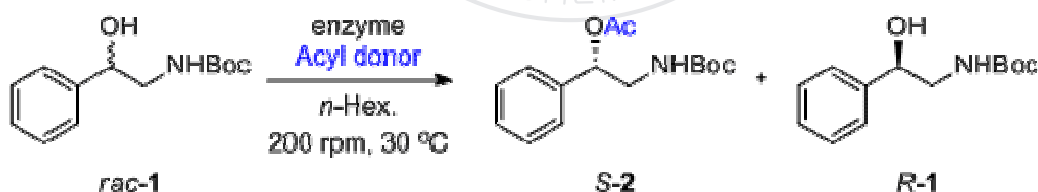
발표종류: 포스터, 발표일시: 금 15:00~17:00

## Kinetic Resolution of Aminoalcohols via Lipase-catalyzed Transesterification

민보라, \*Vani Nelamane Devegowda, \*\*박아름, \*\*\*이혁

성균관대 화학과 \*한국화학연구원 의약화학연구센터 \*\*과학기술연합대학원대 의약 및 약품화학 \*\*\*한국화학연구원 신약연구단

The kinetic resolution of racemic compounds by using enzymes such as lipases and esterases provides one of the most convenient routes to a wide range of enantiomerically enriched molecules including alcohols, acids and their esters. N-Boc protected rac-2-amino-1-phenylethanol rac-1 was synthesized, and several kinds of lipases were screened for the transesterification of this substrate. Several lipases showed high activities and enantioselectivities to afford the corresponding enantioselective ester derived from (S)-2-amino-1-phenylethanol S-2.



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발표코드: IV-ORGN.P-278

발표분야: 유기화학

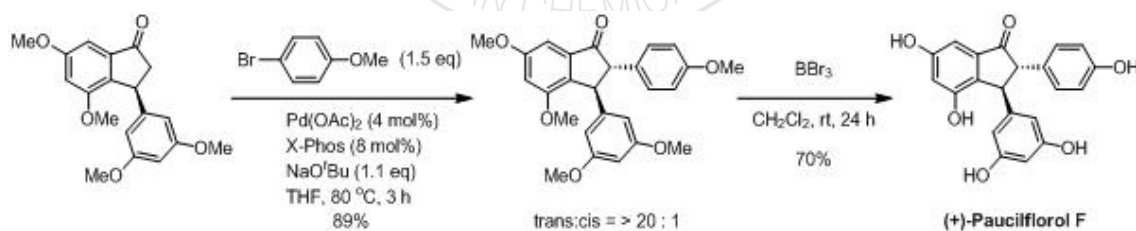
발표종류: 포스터, 발표일시: 금 15:00~17:00

## Stereoselective Palladium-Catalyzed $\alpha$ -Arylation Reactions of 3-Aryl-1-Indanones and Their Application to an Asymmetric Synthesis of (+)-Pauciflorol F

이봉향, \*최영록, 신승훈, \*\*정은영, \*\*허정녕

한양대 화학과 \*고려대 화학과 \*\*한국화학연구원 의약화학연구센터

Pauciflorol F belongs to a large family of polyphenolic natural products including resveratrol and its derivatives, which receive much attention due to interesting biological activities such as anticancer, antibacterial, and anti-HIV. A Highly stereoselective, palladium-catalyzed  $\alpha$ -arylation of 3-aryl-1-indanone with aryl bromide is described. The use of sodium tert-butoxide as a base is important to decrease the undesired products and to increase the stereoselectivity. Ultimately, this methodology successfully applied to the asymmetric synthesis of (+)-pauciflorol F with high efficiency.



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장소: 제주ICC

발표코드: IV-ORGN.P-279

발표분야: 유기화학

발표종류: 포스터, 발표일시: 금 15:00~17:00

## Dialkylammonium Salts and Crown Ether using a new [2]catenane formation

정주미, 이환석, 전남중, 남계춘

전남대 화학과

A very simple self-assembling system, We demonstrate that secondary dialkylammonium salts can thread through the cavity of coumarine crown ether to form [2]pseudorotaxanes. These template-directed syntheses rely on the formation of pseudorotaxane intermediates, which self-assemble in solution from functionalized secondary dialkylammonium hexafluorophosphate threads and macrocyclic polyether rings. These catenane self-assemble from readily available components well-known crown ethers and secondary dialkylammonium hexafluorophosphate salts, have been characterized only in the solid state. Based on this new coumarine crown ether/secondary dialkylammonium salt recognition motif, a [2]catenane was successfully prepared. The formation of these threaded structures was confirmed by  $^1\text{H-NMR}$  spectroscopy.

일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: IV-ORGN.P-280

발표분야: 유기화학

발표종류: 포스터, 발표일시: 금 15:00~17:00

## Fluorescent Chemosensor for Anions Based on Salt Type Derivative

전남중, 홍성원, 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. Fluorescent chemosensors can be effectively used as a tool to analyze and clarify such roles of charged chemical species in living system as well as to measure the amount of ions from the sources contaminated with them. Among anion receptors, colorimetric and fluorescent chemosensors are important because they provide high sensitivity and convenience for monitoring the anion recognition. The salt type derivative was obtained successfully by the reaction of bipyridine with pyrene derivative. The binding properties of pyreneamide derivative investigated with  $^1\text{H}$ -NMR and fluorescence titration methods with various anions.

일시: 2011년 4월 28~29일(목~금) 2일간

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발표코드: IV-ORGN.P-281

발표분야: 유기화학

발표종류: 포스터, 발표일시: 금 15:00~17:00

## **A new selective pyrene containing fluorescence Chemosensor for metal cation**

홍주현, 정주미, 남계춘

전남대 화학과

A new Chemosensor of selective and sensitive models an important role in a wide range of chemical and biological processes. The desired Chemosensor was obtained within minutes through a three-component assembly, involving pyrene unit and crown ether, in which the coordination sphere of metal ion is responsible for metal cations recognition leading to fluorescence enhancement and color change. The Chemosensor formation was characterized by  $^1\text{H}$  NMR and  $^{13}\text{C}$  NMR and UV-vis spectroscopies and color change with various cations.



일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: IV-ORGN.P-282

발표분야: 유기화학

발표종류: 포스터, 발표일시: 금 15:00~17:00

## High Twisted Deep Blue Materials for OLED.

박현태, \*김란, 오대환, \*\*신민기, \*\*\*권순기, 김윤희

경상대 화학과 \*경상대 화학교육과 \*\*경상대 고분자공학전공 \*\*\*경상대 나노신소재공학부

For full-color displays, it is essential to have the three primary colors, red, green and blue. However, compared with green-light-emitting devices, the EL properties of blue-emitting ones need to be improved, particularly in terms of efficiency and color purity, for full-color applications. Excellent blue-emitting materials are important, not only as blue emitters, but also as hosts for dopant emitters to facilitate efficient green and red emission. In this study, we designed and synthesized the anthracene derivatives as high twisted deep-blue light emitting materials. Those high twisted anthracene derivatives possess a non-coplanar that results in a decreased tendency to crystallize and weaker intermolecular interactions in the solid state.

일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: IV-ORGN.P-283

발표분야: 유기화학

발표종류: 포스터, 발표일시: 금 15:00~17:00

## Transition Metal Template Rotaxane and Catenane Synthesis

홍성원, 전남중, 남계춘

전남대 화학과

Topological molecules, catenanes, rotaxanes, knots constitute a major research field in supramolecular chemistry. These molecules display interesting physical properties, such as photoinduced intramolecular electron transfer, electrochemically triggered molecular motions, and photochemical dethreading process. A number of these multicomponent systems have been named 'molecular machines'. Several groups showed ring-closing metathesis (RCM) was extremely useful for catenanes, rotaxanes and knots syntheses. Also, the electron deficient and electron rich components are arranged so that  $\pi$ - $\pi$  stacking is possible. Our approach has been to bring together neutral macrocyclic component and containing positively charged pyridinium axles to create catenane with ring-closing metathesis. The rotaxane and catenane binding properties investigated with  $^1\text{H-NMR}$  and fluorescence titration methods with various Transition metal ions.

일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: IV-ORGN.P-284

발표분야: 유기화학

발표종류: 포스터, 발표일시: 금 15:00~17:00

## Microwave-Assisted Cleavage of Ethers Using an Ionic Liquid

박세경, 채정현

성신여대 화학과

An efficient dealkylation of alkyl aryl ethers using an ionic liquid, 1-n-butyl-3-methylimidazolium bromide ([bmim][Br]) has been developed. Various alkyl aryl ethers are successfully cleaved by the halide anion of [bmim][Br], without aid of any other activating agents. In this reaction, microwave irradiation was found to be crucial for the effective conversion. The newly developed protocol is a very attractive green chemical process as it utilizes minimal amount of cleaving reagents and does not require additional activating agents or solvents. Under the conditions described herein, a broad range of methyl, ethyl, propyl, and benzyl aryl ethers were converted to the corresponding phenolic compounds in good to excellent yields in a short time.

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장소: 제주ICC

발표코드: IV-ORGN.P-285

발표분야: 유기화학

발표종류: 포스터, 발표일시: 금 15:00~17:00

## Identification and Standardization of Bioactive Compounds from Peucedanum Japonicum Thunberg

이정아, 정덕상, 백승준, \*한충훈, 오한솔

제주대 화학과 \*제주대 방사선응용과학연구소

Peucedanum japonicum Thunberg have been used for hypertension, diuresis, suppression and menorrhagia. In this Study, we performed measurement of whitening effect from peucedanum japonicum Thunberg. 70% MeOH extract of peucedanum japonicum Thunberg was fractionated by n-hexane, methylenchloride (MC), ethyl acetate (EA) n-butanol and water, with five fractions, test of inhibition on tyrosinase, test of inhibition on melanin synthesis by using B<sub>16</sub>F<sub>10</sub>melanoma cell were screened to determine whitening activity. As a result, 70% MeOH extract and EA fraction of peucedanum japonicum Thunberg showed to have good qualified activities. Based on this result, components were isolated by activity guided fractionation. In EA fraction of peucedanum japonicum Thunberg, two compounds were 4-(2-hydroxy-1-methoxyethyl)phenol and 7-hydroxy-6-(2,3-dihydroxy-3-methylbutyl)-2H-chromen-2-one (Peucedanol) by physicochemical data spectroscopic methods. To investigate the melanogenesis inhibitory effects of these compounds, the melanin level and tyrosinase activity were examined in B<sub>16</sub>F<sub>10</sub> melanoma cell. Quantitative analysis methods were developed by HPLC. Validation for verification of HPLC methods was carried out to check to specificity, linearity, intra-day precision, inter-day precision and accuracy by ICH guideline. At the same time, quantitative HPLC methods were established to measure content of each standard compounds on extract.

일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: IV-ORGN.P-286

발표분야: 유기화학

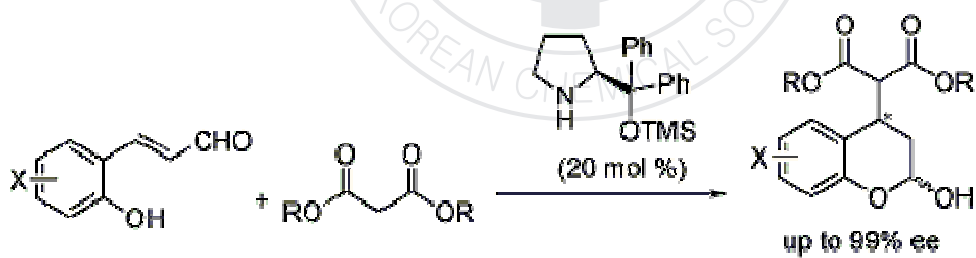
발표종류: 포스터, 발표일시: 금 15:00~17:00

## Asymmetric organocatalytic malonate addition *o*-hydroxycinnamaldehydes: A facile enantioselective access to chromanes

이용천, \*김성곤

경기대 자연과학부 화학과 \*경기대 화학과

Catalytic asymmetric 1,4-addition reactions of malonate to *o*-hydroxycinnamaldehydes, which afford chroman-2-oles, have been established using a diphenylprolinol silylether as catalyst. The chroman-2-oles have been obtained in high chemical yields and enantioselectivities and can be readily used to obtain a variety of chromane derivatives through subsequent transformations.



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발표코드: IV-ORGN.P-287

발표분야: 유기화학

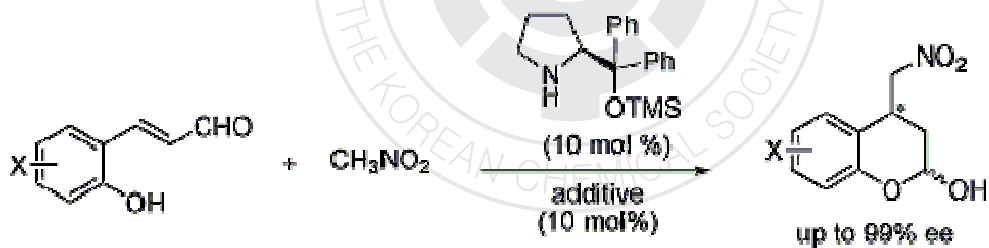
발표종류: 포스터, 발표일시: 금 15:00~17:00

## Enantioselective organocatalytic conjugate addition of nitromethane to *o*-hydroxycinnamaldehydes

최광수, 김성곤

경기대 화학과

Catalytic asymmetric 1,4-addition reactions of nitromethane to *o*-hydroxycinnamaldehydes, which afford 4-substituted chroman-2-oles with high yields and enantioselectivities, have been established using a diphenylprolinol silylether as organocatalyst.



일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: IV-ORGN.P-288

발표분야: 유기화학

발표종류: 포스터, 발표일시: 금 15:00~17:00

## Asymmetric Preparation of D-Phg-L-Pro Dipeptide-derived Chiral Ligands for Enantioselective Addition of Diethylzinc to Aldehyde

강석용, 박용선

건국대 화학과

Optically pure N-aminoethyl prolinol derivatives have been prepared from the dynamic kinetic resolution of N-( $\alpha$ -bromo- $\alpha$ -phenylacetyl) proline ester in asymmetric nucleophilic substitution and subsequent reduction. The D-Phg-L-Pro dipeptide-derived prolinols are tested as chiral ligands in the enantioselective addition of diethylzinc to aldehydes. A N,N-dinaphthylmethyl substituted prolinol chiral ligand has been shown to be effective to produce enantioenriched 1-substituted propanols with up to 95:5 er.

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장소: 제주ICC

발표코드: IV-ORGN.P-289

발표분야: 유기화학

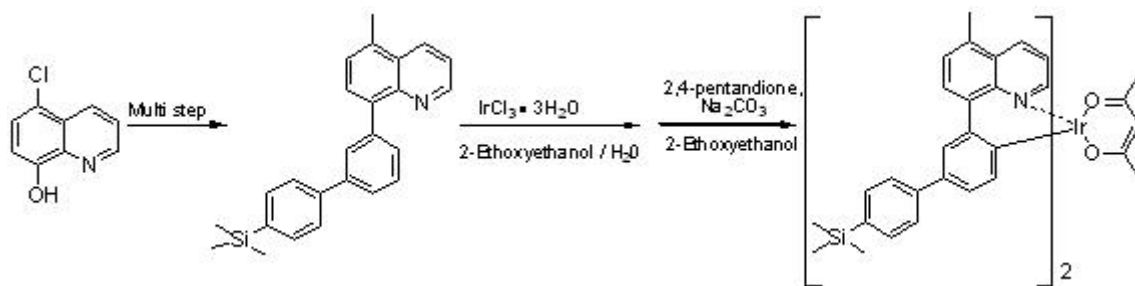
발표종류: 포스터, 발표일시: 금 15:00~17:00

## Synthesis of six-membered chelated iridium coomplex for OLEDs

안진영, 김현진, 정은빈, 황민지, 김윤희, 이상경

경상대 화학과

Last decade, phosphorescence studies of a five-membered chelated iridium(III) complexes have been carried out. But six-membered chelated iridium complexes have not informed about the suitability, the phosphorescent emission high quantum efficiency and maximum brightness comparable to those of five-membered iridium complexes. Few of isoquinoline derivatives were searched for OLED applications and resulted good electroluminescence properties after chelating with metal to form complexes. On the other hand, the compounds included trimethylsilyl(TMS) functional groups shown higher vapor pressure, thermal stability and good solubility. Therefore, the combination of isoquinoline derivatives and bulky trimethylsilyl moieties would be expected to be the best way to achieve an efficient phosphorescent emitter. In this paper, we report the synthetic route and the physical properties of six-membered chelated iridium complex including TMS group.





일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: IV-ORGN.P-290

발표분야: 유기화학

발표종류: 포스터, 발표일시: 금 15:00~17:00

## Highly selectively monitoring heavy and transition metal ions by a fluorescent based on dipeptide

Neupane Lok Nath, 이건형

인하대 화학과

The design and development of fluorescent chemosensor for detection and quantification of low contamination of heavy and transition metal ions (HTM) in water have become significant due to the toxicity of these metal ions to living organisms.. Fluorescent sensor based on amino acid show selective and sensitive response to different metal ions depending on the metal chelating ability of the amino acid for metal ions. Here, we synthesized dansyl labeled dipeptide, Dan-Met-His (DMH) and analyzed the selectivity and sensitivity of different metal ions in 100% aqueous solution. The sensor (DMH) shows only response to Ag(I), Hg(II) and Cu(II) among 13 tested metal ions by three different way. The sensor shows turn on response to Ag(I), ratiometric response to Hg(II) and turn off response to Cu(II) in 100% aqueous system. The detection limit, stoichiometry, binding mode, pH dependent and reversibility of Ag(I), Hg(II) and Cu(II) ions were also studied.

일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: IV-ORGN.P-291

발표분야: 유기화학

발표종류: 포스터, 발표일시: 금 15:00~17:00

## **Ratiometric and selective Fluorescent Sensor for Hg(II) Based on the Pyrene Derivative.**

양미화, 이건형

인하대 화학과

Pyrene labelled methionine is synthesized in solid phase synthesis. The sensor shows highly sensitive and selective response to Hg ions among various metal ions. The sensor sensitively detects Hg(II) ions ratiometrically in aqueous dimethylformamide solution. In the DMF percentages between 2 and 10, This sensor exhibits strong and selective dual fluorescence responses of monomer and excimer to Hg(II). When the DMF percentage exceeded 30, it exhibited a strong monomer emission.

일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: IV-ORGN.P-292

발표분야: 유기화학

발표종류: 포스터, 발표일시: 금 15:00~17:00

## **A ratiometric fluorescent sensor based on dipeptide for Ag( I ) with high selectivity and sensitivity.**

장수정, 이건형

인하대 화학과

Pyrene fluorophore were conjugated with Trp and His amino acid in solid phase synthesis. This sensor detected Ag( I ) in a 100% aqueous solution with high sensitivity via ratiometric response. and Reaction of sensor with Ag( I ) leads to formation of pyrene excimer. It is concluded that the fluorescence response of the sensor results from the formation of 2:1 complex and 1:1 complex mixed type with the metal ion.

일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: IV-ORGN.P-293

발표분야: 유기화학

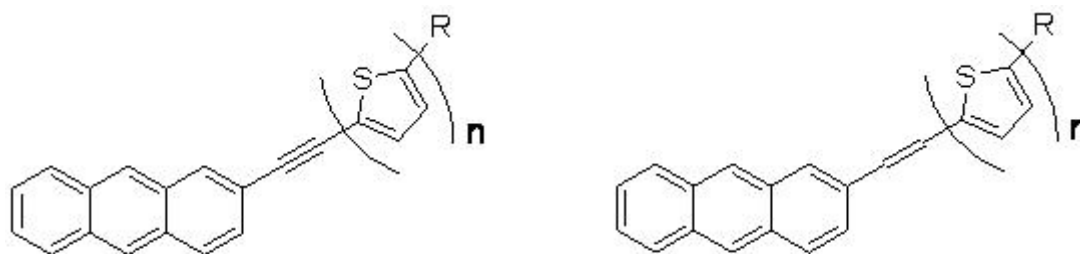
발표종류: 포스터, 발표일시: 금 15:00~17:00

## Synthesis and Characterization of Anthracene Derivatives for OTFTs

황민지, 안진영, 김현진, 임기범, 정은빈, 이상경

경상대 화학과

Recently, organic thin film transistor (OTFT) has drawn great attention because of its advantages over conventional inorganic electronics such as low cost, facile packaging, and compatibility with flexible substrates. These advantages are essential for display operation of next generation such as organic light-emitting diode (OLED), low cost identification tags and flexible sensor. But the OTFTs have lower mobility and switching speeds compared to silicon semiconductors. In the recent studies, the asymmetrically alkylated compound exhibited up to  $0.3 \text{ cm}^2 / (\text{Vs})$  p-type charge carrier mobility. In a thin film phase, unlike the symmetrically substituted compounds, the asymmetrically substituted compounds showed nearly vertically. Because of the different alignment give a measurable effect on the charge transport. For this reason, we designed a series of asymmetric anthracene derivatives, and synthesized for studies of characterization. Then, we compared characterization of synthesized compounds 1 and 2 which has same substituted acene and aliphatic groups except  $\text{C}=\text{C}$  and  $\text{C}\equiv\text{C}$ .



$n = 1, 2$

$R = -\text{C}_6\text{H}_{13}, -\text{C}_{12}\text{H}_{25}$

일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: IV-ORGN.P-294

발표분야: 유기화학

발표종류: 포스터, 발표일시: 금 15:00~17:00

## Synthesis of Sulfonamides

정은빈, 안진영, 김현진, 임기범, 황민지, 이상경

경상대 화학과

Antibiotics are chemical substances extremely active at low doses that kill or slow the growth of bacteria. Among of the antibiotics, sulfonamides are the best well known structure and studied for long times. In the past decades, the studies of sulfonamides in science field slowly changed because of the utility of sulfonamides were become diversity. That means the utility of sulfonamides not only focused on the use of antibiotics but also used for the other purpose such as studies of immunoassay, glycerol 3-phosphate acyltransferase (GAPT) and antiobesity. On this presentation, we want to report very simple sulfonamides which were synthesized in our laboratory for aid of other researchers such as immunoassay and antiobesity.

일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: IV-ORGN.P-295

발표분야: 유기화학

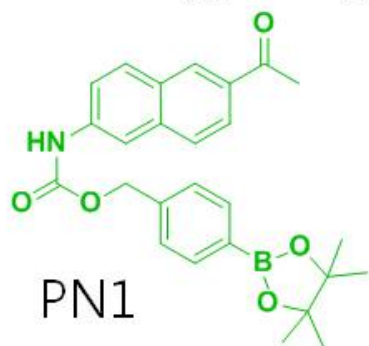
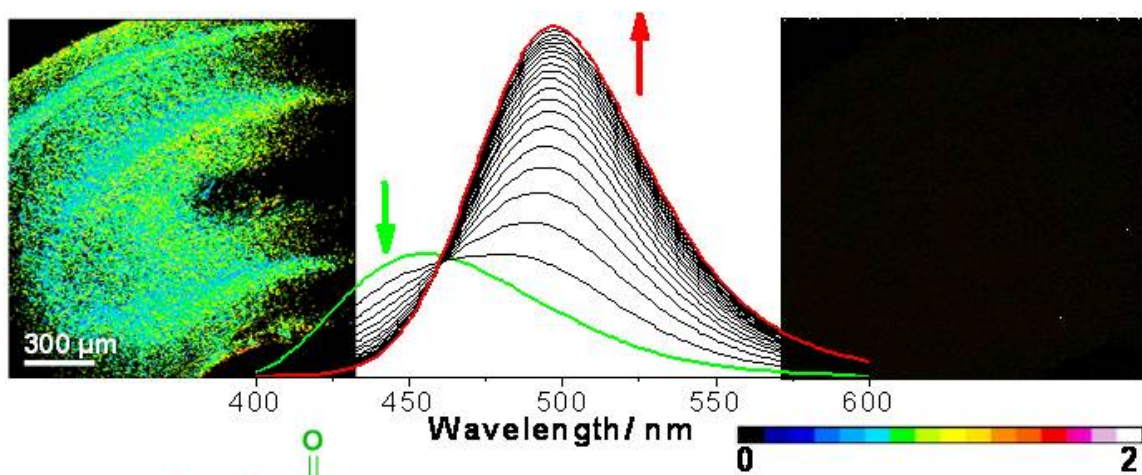
발표종류: 포스터, 발표일시: 금 15:00~17:00

## A Two-Photon Fluorescent Probe for Ratiometric Imaging of Hydrogen Peroxide in Live Tissue

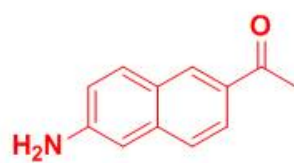
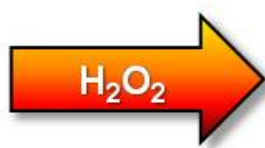
정 철, 장민경, 조봉래

고려대 화학과

Hydrogen peroxide ( $\text{H}_2\text{O}_2$ ) is a prominent member of the reactive oxygen species (ROS) family that includes superoxide anion radical ( $\text{O}_2^\bullet$ ), hydroperoxy radical ( $\text{HO}_2^\bullet$ ), hydroxyl radical ( $\text{HO}^\bullet$ ), peroxy radical ( $\text{RO}_2^\bullet$ ), singlet oxygen ( $^1\text{O}_2$ ), and hypochlorous acid ( $\text{HOCl}$ ), and plays important roles in physiology, aging, and disease in living organisms. Unregulated increases in cellular levels of  $\text{H}_2\text{O}_2$  have been linked to DNA damage, mutation, and genetic instability, whereas controlled bursts of  $\text{H}_2\text{O}_2$  are utilized for cell signaling. We now report a new type of ratiometric TP fluorescence probe for  $\text{H}_2\text{O}_2$ , Peroxy Naphthalene 1 (PN1), by introducing a boronate-based carbamate leaving group to the two-photon fluorophore 2-acetyl-6-aminonaphthalene (AN1), with the expectation that the  $\text{H}_2\text{O}_2$ -triggered boronate cleavage of the electron-poor carbamate linkage would liberate the more electron-rich AN1 and result in a red-shifted fluorescence. We adopted AN1 as the fluorophore reporter because TP probes derived from this dye have been successfully utilized in live tissue imaging



PN1



AN1



일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: IV-ORGN.P-296

발표분야: 유기화학

발표종류: 포스터, 발표일시: 금 15:00~17:00

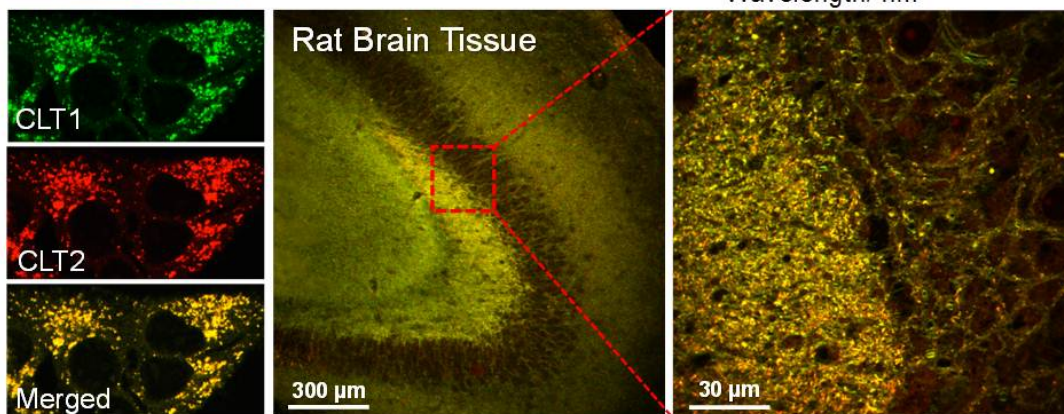
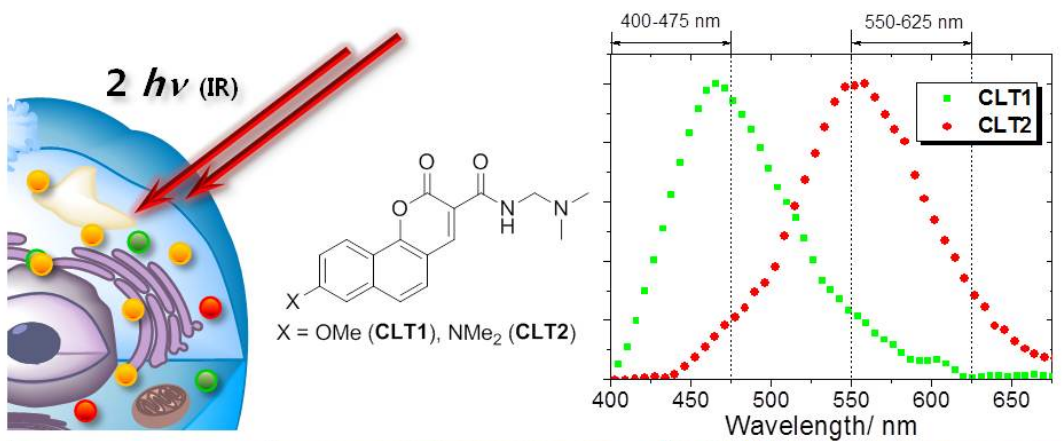
## Two-Photon LysoTrackers for In Vivo Imaging

임창수, 이정화, Muhammad Nawaz, 조봉래

고려대 화학과

Lysosomes are acidic organelles that constitute the terminal degradative compartments in the mammalian cells. They receive and degrade macromolecules through the phagocytic, endocytic, and autophagic pathways, and play vital roles in various physiological processes. To understand their roles in physiology, a variety of fluorescent lysosomal probes have been developed with some of them being commercially available. However, use of these probes with one-photon microscopy (OPM) required excitation with short-wavelength light (~350–550 nm) that limited their application in deep tissue imaging. Overcoming these problems requires the development of two-photon (TP) probes that can detect lysosomes in live cells and tissues by using two-photon microscopy (TPM). TPM, which uses two photons of lower energy for the excitation, is a new technique that can visualize deep inside intact tissues noninvasively for an extended period of time. However, TP probes for lysosomes are rare. We have employed chromene as the fluorophore because it showed significant TP cross section, introduced different donors to tune the emission wavelengths, and ethylenediamine moiety as the proton binding site. We have now developed chromene-derived lysosomal TP probes that emit fluorescence in the blue (CLT1) and yellow (CLT2) regions. The spectroscopic studies conducted in universal buffer reveal that CLT1 and CLT2 show absorption maxima at 389 and 449 nm, and fluorescence maxima at 447 and 580 nm, respectively.





일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: IV-ORGN.P-297

발표분야: 유기화학

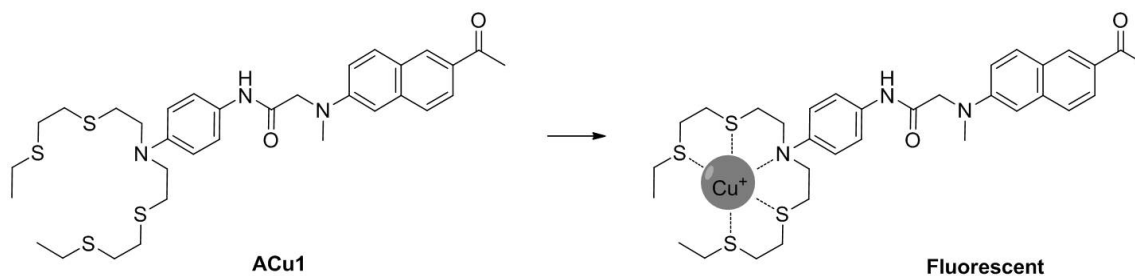
발표종류: 포스터, 발표일시: 금 15:00~17:00

## A Two-Photon Probe for Copper(I) Ions in Live Cells and Tissues

임창수, Sajal Kumar Das, 조봉래

고려대 화학과

Copper is an essential element for life, but alterations in its cellular homeostasis are connected to serious neurodegenerative diseases, including Menkes and Wilson diseases, familial amyotrophic lateral sclerosis, Alzheimer's disease, and prion diseases. Because of its essential yet toxic nature, cells exert strict control over intracellular copper distributions, and the thermodynamically estimated level of free copper in the cytosol of bacterial modelsystems is less than one ion per cell. We synthesize  $\text{Cu}^+$  selective two photon fluorescent probes (ACu1) with dissociation constants ( $K_d^{\text{TP}} = 113 \pm 9 \text{ pM}$ ). They show appreciable water solubility ( $> 3 \text{ }\mu\text{M}$ ), cell permeability, high photostability, pH insensitivity at  $\text{pH} > 7$ , significant two-photon action cross sections (100 GM) upon complexation with  $\text{Cu}^+$ , and can detect the  $\text{Cu}^+$  in the HeLa cells and in the living mouse hippocampal slices at a depth of  $> 80 \text{ }\mu\text{m}$  without mistargeting and photobleaching problems.



일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: IV-ORGN.P-298

발표분야: 유기화학

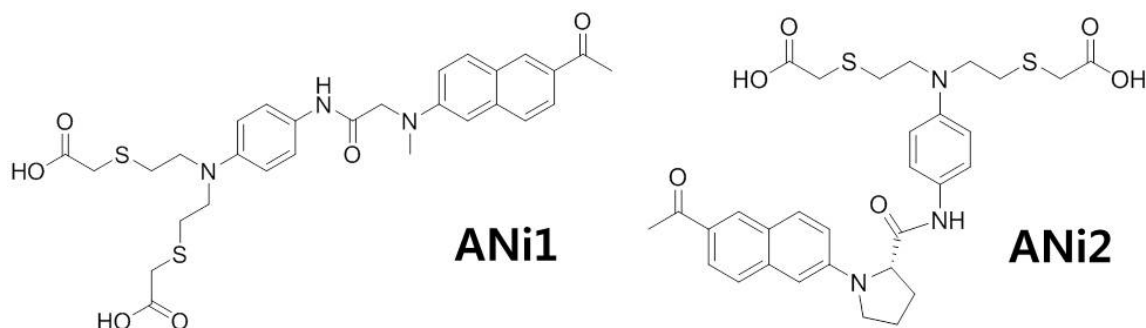
발표종류: 포스터, 발표일시: 금 15:00~17:00

## Detection of Nickel in Fish Organs with a Two-Photon Fluorescent Probe

한지희, \*김창우, \*박희정, \*조봉래

고려대 화학 \*고려대 화학과

Nickel is used in many industrial and consumer products including, magnets, coinage, and special alloys. Nickel enters environment via both natural and human activities. The toxicity of nickel is low but excess nickel accumulation can cause lethal effects in the aquatic ecosystems. The fishes living in the polluted water can take  $\text{Ni}^{2+}$  through mouth and skin, which can be accumulated in different organs. Among the sea food, salmon (1.70 ppm), oysters (1.50 ppm), and clams (0.58 ppm) have the highest nickel contents. According to US EPA, the average intake of nickel by American adults ranges from 300 to 600  $\mu\text{g}/\text{day}$ . To detect  $\text{Ni}^{2+}$  inside the fish organs, it is crucial to use two-photon microscopy (TPM). TPM, which utilizes two photons of lower energy for the excitation, has the advantages of increased penetration depth ( $> 500 \mu\text{m}$ ), localized excitation, and prolonged observation time, thereby allowing deep tissue imaging. 1 derived from 1 have been successfully utilized in live tissue imaging and CTEA as the receptor for  $\text{Ni}^{2+}$  from the work of previous workers. So we synthesized ANi1 and ANi2 for detect  $\text{Ni}^{2+}$ .



일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: IV-ORGN.P-299

발표분야: 유기화학

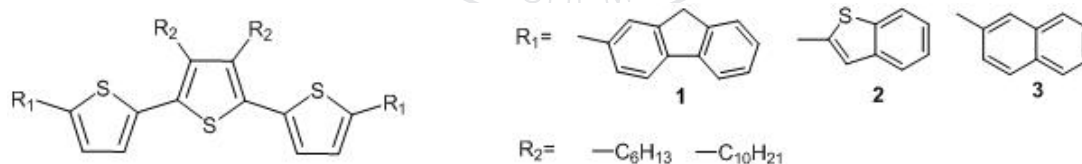
발표종류: 포스터, 발표일시: 금 15:00~17:00

## Synthesis and physical properties of OFETs including terthiophene in core.

김현진, 정은빈, 황민지, 안진영, 임기범, 이상경

경상대 화학과

Conjugated oligomers have attracted intense interest in recent years from both academic and industrial communities. The ease of producing materials with well-defined molecular structures and high purity renders them promising candidates as the active materials in thin-film optoelectronic devices such as organic field-effect transistors (OFETs). Semiconducting small molecules include the polycyclic aromatic compounds such as pentacene, anthracene, and rubrene. In here, we presented a new structure of OFET candidates which synthesized by our research members. The synthesized materials were designed based on increasing solubility by introduced long chain alkyl group at the core of the material.



일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: IV-ORGN.P-300

발표분야: 유기화학

발표종류: 포스터, 발표일시: 금 15:00~17:00

## Preparation of Chlorotetrazole as a Ligand for Green Primary Explosive Metal Complexes

문석식, 유현아, \*김연철, 이석우

공주대 화학과 \*공주대 고분자공학과

Recently, environment-friendly complexes of cobalt, iron, zinc, and copper with nitrogen-rich tetrazole analogues have been of great interest in a sense that they might replace some harmful metal-based explosives like lead azide, lead styphnate, mercury fulminate, which have been used for primary explosives. For example, a cobalt complex with nitrotetrazole (BNCP) have been reported to show excellent safety properties like friction sensitivity, electrostatic discharge, spark sensitivity, and impact sensitivity. Chlorotetrazole have been utilized as a ligand for a cobalt metal. However, its preparation from aminotetrazole or nitrotetrazole has been a problematic matter due to low yield and explosion. Here, we present a safe and high yielding procedure for preparation of chlorotetrazole and its sodium salt.

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발표분야: 유기화학

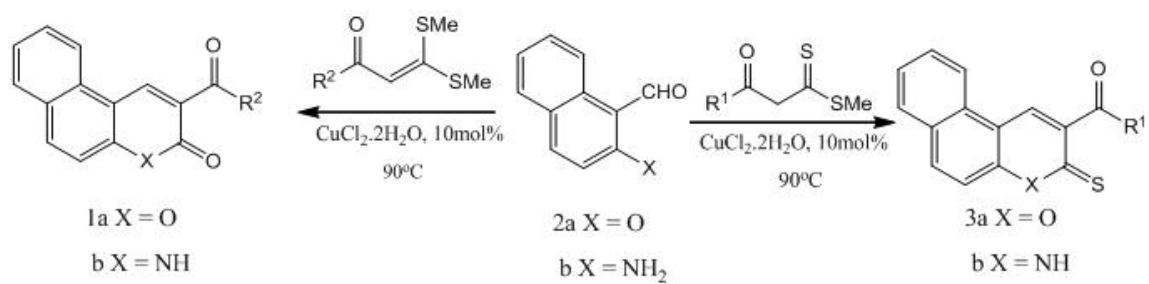
발표종류: 포스터, 발표일시: 금 15:00~17:00

## Facile Synthesis of Various Coumarin and Benzo[f]quinolinone Derivative Under Solvent Free Condition

임기별, 김현진, 황민지,정은빈, 안진영, 이상경

경상대 화학과

Many classical routes have been available for the synthesis of coumarin and benzo[f]quinolinones. The Pechmann reaction for the synthesis of coumarin involves the condensation of phenols with  $\beta$ -ketonic esters in the presence of variety of acidic condensing agents such as sulphuric acid, hydrochloric acid and phosphoric acid, phosphorous pentoxide, trifluoroacetic acid and Lewis acids such as  $ZnCl_2$ ,  $AlCl_3$  and exchange resins, have also been used. In recent year, conventional method for syntheses of coumarin and benzo[f]quinolinones derivative include the Au(I)-catalyzed intramolecular hydroarylation of terminal alkynes, intermolecular cyclization of o- hydroxycinnamaldehyde, ortho-substituted cinnamate and N-phenylacrylamide. However these methods not only suffer disadvantages from using a large excess of expensive transition-metal and harsh condition but also unfriendly environment. We have successfully demonstrated the facile synthesis of two different coumarin derivatives by the reaction of 2-hydroxy-1-naphthaldehyde with easily accessible  $\beta$ -oxodithioester and S,S-acetal in the presence of catalytic amount of  $CuCl_2$  under solvent free condition. This scheme offers a good scope for the synthesis of a wide variety of fused heterocyclic arenes.



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장소: 제주ICC

발표코드: IV-ORGN.P-302

발표분야: 유기화학

발표종류: 포스터, 발표일시: 금 15:00~17:00

## **Photo-curable propyl cinnamate functionalized polyhedral oligomeric silsesquioxane (POSS) as a gate dielectric for organic thin film transistors.**

김윤택, 황도훈

부산대 화학과

Organic field-effect transistors (OFETs) consist of a gate insulator and an organic semiconductor. In recent years, performances of organic semiconductors have been improved considerably, but insulating materials are still a weak link in OFETs. Here we synthesized polyhedral oligomeric silsesquioxane (POSS)-based photo-curable insulating materials with propyl cinnamate groups. The synthesized insulators were cross-linked and solidified under UV irradiation. We fabricated MIM device of ITO/insulator/Au to measure electrical properties such as leakage current and capacitance of the materials. We also fabricated an organic thin film transistor (OTFT) using pentacene as an active p-type organic semiconductor and the synthesized insulator as a gate dielectric layer. Properties of insulating materials and device characteristics of OTFTs will be presented.



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발표코드: IV-ORGN.P-303

발표분야: 유기화학

발표종류: 포스터, 발표일시: 금 15:00~17:00

## Composition Analysis on Essential Oil and Floral Water of Hallabong Tangor (Citrus kiyomi × ponkan)

이정아, \*한충훈, 정덕상, 변종철, 이선주, 현동림, 양영진

제주대 화학과 \*제주대 방사선응용과학연구소

Aroma therapy has been generally used to the public doesn't feel strange when they hear about it, as it has been expanding its application areas to alternative medicine not to mention about skin treatment. The chemical contents of essential oil used for the aromatherapy may depend on many reasons, and they have become meaningful factors to decide the perfume and effect of each aroma oils. The chemical compositions of the oil and floral water constituents from Hallabong tangor (Citrus kiyomi × ponkan) and lemon were determined GC/MS spectrometric analysis with Wiley Library searches. The major constituents identified were as dl-Limonene (84.71%),  $\beta$ -Myrcene (7.00%),  $\alpha$ -Terpineol (4.62%), Terpinene-4-ol (3.67%) in Hallabong tangor oil.

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장소: 제주ICC

발표코드: IV-ORGN.P-304

발표분야: 유기화학

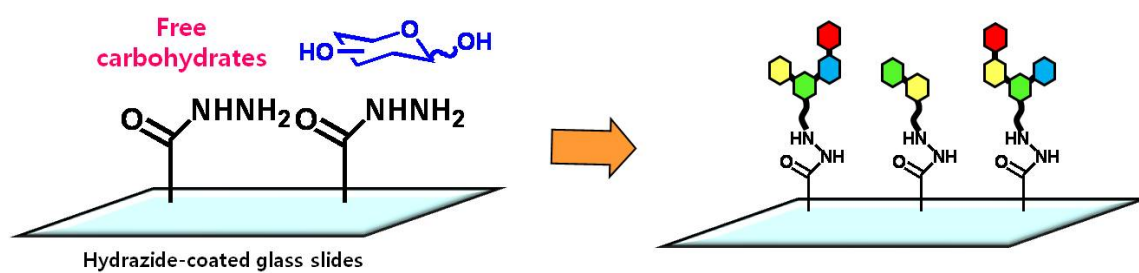
발표종류: 포스터, 발표일시: 금 15:00~17:00

## **A novel, direct, site-specific technique for immobilization of unmodified carbohydrates on hydrazide-derivatized surfaces**

배재영, 신인재

연세대 화학과

Carbohydrate-protein recognition events play key roles in physiological and pathological processes. The understanding of these biomolecular interactions provides deep insight into glycan-mediated biological processes and enables the development of more effective therapeutic agents and diagnostic tools. Carbohydrate microarrays, which are composed of diverse glycans orderly and densely attached to a single chip substrate, have been extensively developed as reliable and efficient tools for the rapid analysis of carbohydrate-based biomolecular interactions. The most general method for construction of these microarrays involves site-specific and covalent immobilization of chemically modified glycans to properly derivatized surfaces. This immobilization strategy requires the use of properly functionalized sugars, which are typically prepared by multi-step synthetic sequences. In order to avoid the need for functionalized glycans, immobilization strategies that employ unmodified sugars have been developed. In recent investigations directed at this goal, we have developed a novel, direct, site-specific technique for immobilization of unmodified carbohydrates, including simple carbohydrates, oligosaccharides and polysaccharides, on hydrazide-derivatized surfaces. This method eliminates the need for laborious and tedious glycan derivatization. To demonstrate the scope and applicability of this approach, carbohydrate microarrays containing a variety of glycans have been constructed by using one-step, direct attachment of free carbohydrates to a hydrazide-coated surface. These microarrays have been employed for analysis of sugar binding specificities of lectins, antibodies and bacterial cells. In addition, this microarray format has been applied to the determination of binding affinities between proteins and glycans



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장소: 제주ICC

발표코드: IV-ORGN.P-305

발표분야: 유기화학

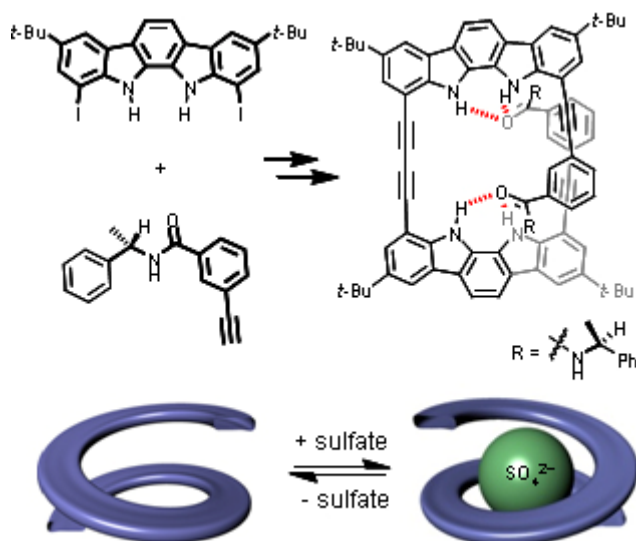
발표종류: 포스터, 발표일시: 금 15:00~17:00

## Molecular Switches Based on the Helical Sense Switching by Anion Stimulus

석재민, 정규성

연세대 화학과

Chiroptical molecular switches comprising indolocarbazole and chiral (*S*)-phenyl-(or naphthyl) ethyl amido units were prepared which folded into a helical conformation by intra-molecular hydrogen bonds. The circular dichroism (CD) spectroscopy showed strong negative Cotton effect, indicative of the left-handed (*M*) helix prevailing over the corresponding right-handed (*R*) helix. Addition of anions such as sulfate led to opposite induced circular dichroism (ICD), suggesting that the helical sense be completely switched from *M*- to *P*-helix upon anion binding. The absolute helical sense of the sulfate complexes was also proved by single crystal X-ray analysis which was consistent with the CD analysis and 2D NOE experiments. Details will be described in the presentation



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발표코드: IV-ORGN.P-306

발표분야: 유기화학

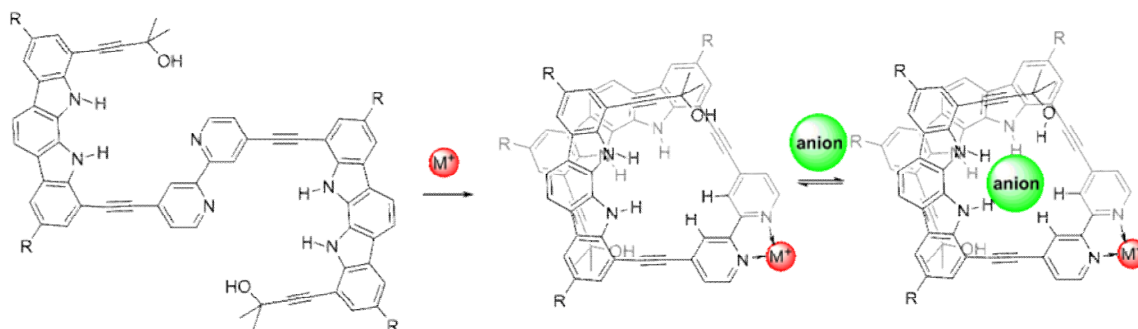
발표종류: 포스터, 발표일시: 금 15:00~17:00

## Cooperative Binding of Anions Induced by Transition Metal Coordination

이현지, 정규성

연세대 화학과

An anion receptor which possess two binding sites linked by 2,2'-bipyridyl spacer has been prepared. Each of the binding sites comprises three convergent hydrogen donors, two NHs and one OH. Because 2,2'-bipyridyl unit exists in a s-trans form due to the dipole-dipole repulsion, two binding sites are located in the opposite side and the cooperative anion binding of the two sites is not possible unless the single bond in between two pyridyls rotates. This process requires large penalty in the binding energy. The chelation of a transition metal to the 2,2'-bipyridyl not only makes two binding sites located in the same side for cooperative binding of anions but also some of aromatic C-H protons enable to participate in hydrogen bonding with anions. As the consequence, the binding affinity and selectivity towards large anions greatly increase and details will be presented in the poster.



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장소: 제주ICC

발표코드: IV-ORGN.P-307

발표분야: 유기화학

발표종류: 포스터, 발표일시: 금 15:00~17:00

## **Phenylurea-based anion receptors capable of transporting chloride through lipid membranes**

최예린, 정규성

연세대 화학과

Membrane transport of anions is an important biological process which is closely associate with a variety of severe diseases. The example includes cystic fibrosis caused by mutations in the cystic fibrosis transmembrane conductance regulator (CFTR) Cl<sup>-</sup> channel. This gives rise to a variety of diseases including severe lung disease, intestinal blockage, male infertility and salty sweat. In the CIC channel, the chloride ion travels with the stabilization by four hydrogen bonds with two NHs and two OHs. We here have designed and synthesized anion receptors that are based on the phenyl urea skeleton and possess the same functional groups with the CIC chloride channel. With these receptors examined are the anion binding properties and transporting activities through a lipid bilayer membrane. Details will be described in the presentation.

일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: IV-ORGN.P-308

발표분야: 유기화학

발표종류: 포스터, 발표일시: 금 15:00~17:00

## Synthesis and Characterization of Aryl Fullerene Derivative for Use in Organic Solar Cells

김희운, \*진성호, 황도훈

부산대 화학과 \*부산대 화학교육과

An aryl fullerene derivative was synthesized through Tosylhydrazone route with C<sub>60</sub> and used as an electron acceptor material for P3HT-based bulk heterojunction solar cells. The new synthesized fullerene derivative showed good solubility in common organic solvents. Optical and electrochemical properties of the new synthesized fullerene were characterized by <sup>1</sup>H NMR, <sup>13</sup>C NMR, UV-vis, DSC, TGA and Cyclic Voltammetry. Photovoltaic devices were fabricated using the configuration as follows ITO/PEDOT:PSS/P3HT:Acceptor/LiF/Al. The UV-vis absorption spectrum was similar to that of PCBM. And the electrochemical measurements showed that new synthesized fullerene has the LUMO levels of -3.72 eV.

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발표분야: 유기화학

발표종류: 포스터, 발표일시: 금 15:00~17:00

## Molecular Iodine Mediated Oxidation and Ring Rearrangement: A Short and Mild Route for the Synthesis of Spiro(benzofuran-2,1'-isobenzofuran)-3,3'-diones

Yashwardhan Malpani, \*정희춘, \*\*김필호, \*\*\*정영식, \*\*\*\*오금록

과학기술연합대 의학 약품화학 \*한국화학연구원 \*\*한국화학연구원 난치성질환치료제연구센터  
\*\*\*한국화학연구원 신물질연구단 \*\*\*\*충남대 화학과

Molecular iodine is useful for numerous organic transformations such as deprotection, idolactonisation and oxidation due to its unique reactivities and association with mild reaction conditions. The molecular iodine mediated oxidations are well known for the conversion of alcohols to ketones. Also, it has been reported that vicinal diols can be oxidized with sodium periodate. However, to the best of our knowledge, no work has been reported for the oxidation of diols with molecular iodine. Spiro lactone structural motifs are known to be present in various natural products such as cochinchistemoninone, saxorumamide, biyouyanagin A, and hyperlactones C. The preparative methods for these spiro lactones generally accompany lengthy synthetic steps and highly acidic or basic conditions which limit the functional group compatibility. Thus, it would be useful to develop a novel synthetic method to prepare spiro compounds. While exploring the synthesis of polycyclic benzofurans, we have developed the first use of molecular iodine in alcoholic solutions for the oxidation and subsequent ring rearrangement which in turn leads to an efficient synthesis of spiro lactones starting from ninhydrin in just two synthetic steps. This gives an access to spiro lactones which can be further utilized. It is important to note that some spiro benzofurans act as fluorogens for the detection of primary amino functionality. Our route could give an easy access to the synthesis of fluorogens and also could increase the functional group compatibility.



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발표코드: IV-ORGN.P-310

발표분야: 유기화학

발표종류: 포스터, 발표일시: 금 15:00~17:00

## Alkyl Phosphate Functionalized Gold Nanoparticles- Based Colorimetric Probe for $\text{Pb}^{2+}$ ions

김수덕, 김승경, 한민수

중앙대 화학과

Phos-AuNPs is an effective colorimetric probe for  $\text{Pb}^{2+}$ . The proposed Probe can detect  $\text{Pb}^{2+}$ , both spectrophotometrically and visually, in aqueous solutions at physiological pH with high selectivity toward  $\text{Pb}^{2+}$  over a variety of metal ions. Moreover, the selectivity is retained even in the presence of other metal ions. In addition, this AuNP-based method has a low detection limit as low as fluorescent chemosensor.

일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: IV-ORGN.P-311

발표분야: 유기화학

발표종류: 포스터, 발표일시: 금 15:00~17:00

## Quencher free oligonucleotide fluorescent chemosensor for Pb(II)

염민식, 한민수

중앙대 화학과

Oligonucleotide 를 기반으로 한 형광센서의 구조는 일반적으로 형광단과 소광단으로 구성되어 있다. 하지만 본 연구에서는  $Pb^{2+}$ 이온이 G-rich Oligonucleotide 와 강하게 결합하여 G-quadruplex 형태를 형성하는 특성을 이용하여 Complex 형성을 유도 하였고, 이 Complex 자체가 효율적인 소광단임을 알 수 있었다. 이를 이용하여 형광단과 소광단을 모두 부착하여 사용하는 종래의 방법과는 다르게 형광단만을 표지한 Oligonucleotide 를 사용하는 보다 단순화된 형태의 Oligonucleotide 를 이용하여  $Pb^{2+}$ 를 효율적으로 검출할 수 있었다. 이 센서는 중성 수용액에서 다른 양이온들에 대하여  $Pb^{2+}$ 이온에 매우 높은 선택성과 3nM 수준의 매우 높은 검출 한계를 가진다.

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발표종류: 포스터, 발표일시: 금 15:00~17:00

## **Colorimetric sensing probe for calcium ions using CTP stabilized gold nanoparticle : colorimetric selective detection of calcium ions over magnesium ions in aqueous solution at physiological pH**

김수덕, 한민수

중앙대 화학과

CTP stabilized-AuNPs (CsAuNPs) were prepared by mixing CTP and citric acid stabilized AuNPs and the AuNPs were proved as a colorimetric selective probe for  $\text{Ca}^{2+}$ . The sensing mechanism of the probe was evaluated by UV-Vis spectrometry and transmission electron microscopy. The studies showed that  $\text{Ca}^{2+}$  ions interconnected CTPs on AuNP to CTPs on other AuNPs and caused them to aggregate, which resulted in a visible color change in the AuNPs solution. The probe could detect  $\text{Ca}^{2+}$  ions in aqueous solution at physiological pH, either spectrophotometrically or visually, with high selectivity towards  $\text{Ca}^{2+}$  ions various metal ions including  $\text{Mg}^{2+}$ . This probe allows a quantitative assay of  $\text{Ca}^{2+}$  down to a concentration of  $10^{-4}$  M and the detection range of this probe also can be tuned easily by changing concentrations of CTP. This probe is working in broad range of pHs between pH 5 to pH 8.

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발표분야: 유기화학

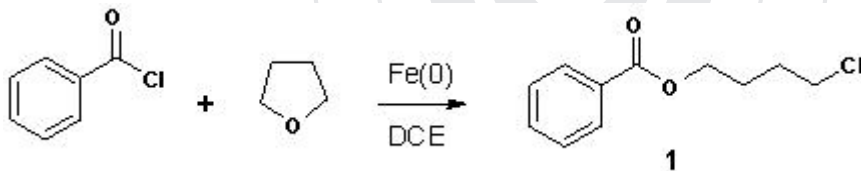
발표종류: 포스터, 발표일시: 금 15:00~17:00

## Fe-mediated synthesis of chloroester moieties

최경민, 정해동, 원태진, 신동수

창원대 화학과

A mild and an efficient synthesis of chloroesters is described by the reaction of cyclic and acyclic ethers with acid chlorides in the presence of Fe(0), affording the corresponding chloroesters in excellent yields. 4-Chlorobutyl benzoate, **1** was prepared by the reaction of tetrahydrofuran and benzoyl chloride in DCE was added Fe(0). The more detailed reaction methodology will be discussed.



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발표분야: 유기화학

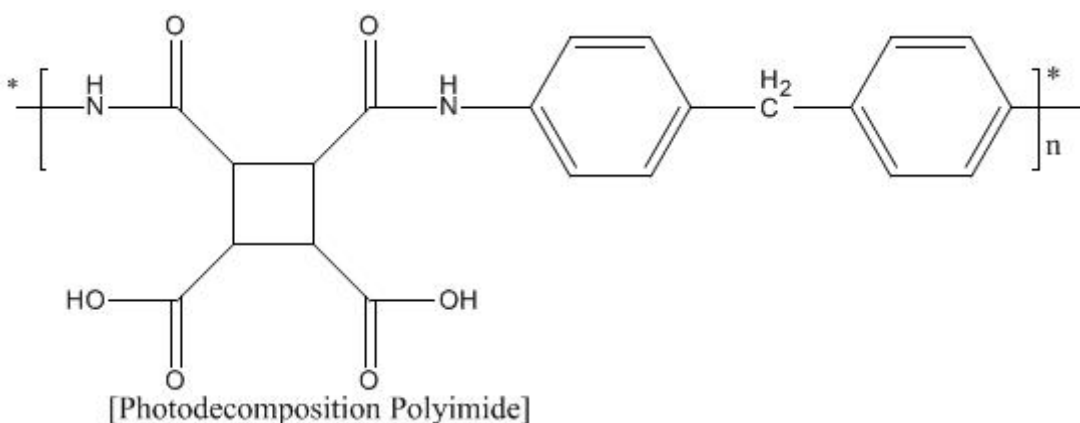
발표종류: 포스터, 발표일시: 금 15:00~17:00

## Photoalignment using Reactive Monomers added Photodecomposition Polyimide

김호중, 신동명

홍익대 화학공학과

Reactive monomer added photodecomposition polyimide film are exposed to linearly polarized UV. After irradiation, polyimide film gives LC alignment, perpendicular to polarization direction of the UV irradiation. LC aligning direction is measured by polar diagram. We had time to adjust during 10min-1hour. And We exposed to linearly polarized UV the angle vertically or horizontally by measured the degree of LC alignment. We studied that effect of polarized UV light on rubbed polyimide film. Anchoring energy of liquid crystal with aligning surface was measured. Irradiation of polarized UV light on rubbed Polyimide film suppressed effective anchoring energy. Linearly polarized UV light on rubbed polyimide film controlled anchoring energy effectively.



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장소: 제주ICC

발표코드: IV-ORGN.P-315

발표분야: 유기화학

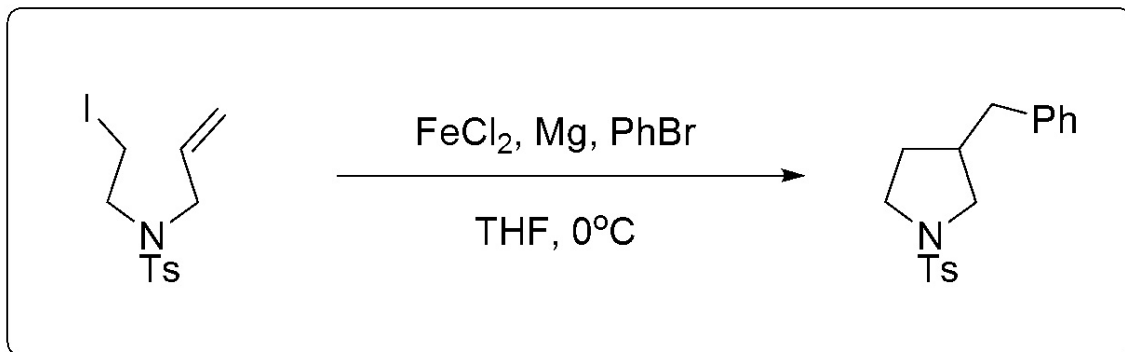
발표종류: 포스터, 발표일시: 금 15:00~17:00

## Fe-Catalyzed Tandem Cyclization/Cross-coupling Reaction

손영훈, 김재곤, 강은주

경희대 응용화학과

The radical reactions of alkyl halide have been well-known as carbon-carbon bond formation reactions. In spite 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.



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발표분야: 유기화학

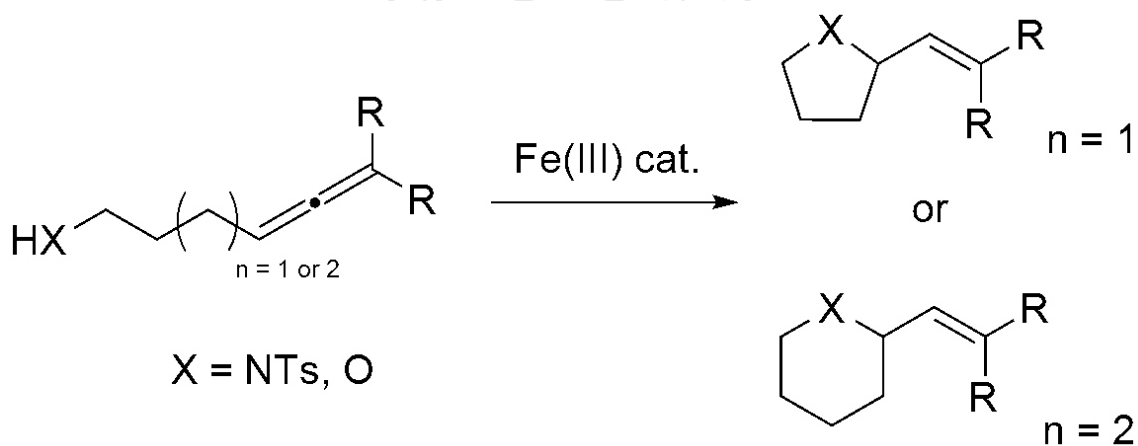
발표종류: 포스터, 발표일시: 금 15:00~17:00

## Fe(III)-catalyzed Hydrofunctionalization of Allenes

정민석, 김원선, 강은주

경희대 응용화학과

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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발표종류: 포스터, 발표일시: 금 15:00~17:00

## Synthesis of DNA-Organic Molecule-DNA Triblock Oligomers And their Amplification Using the PCR Method

정영환, \*Jungkyu K. Lee, \*Zhenan Bao

한국폴리텍바이오대학 바이오생명정보과 \*Stanford University, U.S.A.

Molecular electronics, which involves molecular building blocks as active electronic elements, has been the subject of intense research for many years because of the fundamental interests in molecular charge transport and potential applications. Molecular electronics requires a method for making reliable electrical contacts to single-molecules. DNA has been used as a template for metallic nanostructures, such as Ag, Au, Pd, and Cu nanowires. We envision using a DNA-organic molecule-DNA (DOD) triblock architecture, where the DNAs are subsequently “metallized” to enable contacts to a single molecule. Long double strand DNAs (dsDNAs) (>a few-hundred nanometers) are needed to tether individual molecules to lithographically patterned microscopic electrodes. As a key first step, we demonstrate the synthesis of such triblock adducts and their subsequent elongation to construct molecular electronic suitable DOD architectures using polymerase chain reaction (PCR). We have successfully developed a simple and versatile approach using PCR to synthesize triblock architectures comprising “long dsDNA-organic molecule-long dsDNA.” The amide-coupling reactions allowed us to incorporate molecules with 3'-ODN end substitutions and can be easily extended to introduce other organic molecules to build various ODN nanostructures, for example three-armed ODN nanostructures. Moreover, the PCR method is a powerful tool to rapidly build micrometer-scaled DNA structures from the ODN precursors. By incorporating organic molecules with interesting electronic properties, this strategy could constitute a versatile biomolecule-based platform for single molecule electronics.



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발표코드: IV-ORGN.P-318

발표분야: 유기화학

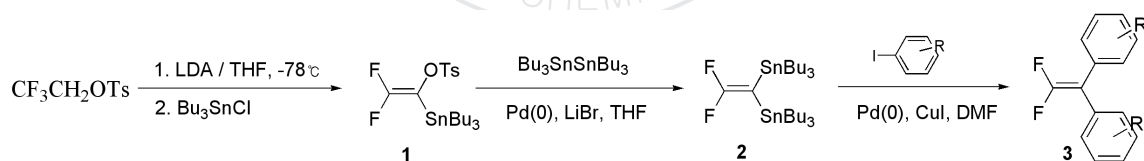
발표종류: 포스터, 발표일시: 금 15:00~17:00

## Preparation of (2,2-Difluoroethene-1,1-diyl)bis(tributylstannane) and its arylation reaction

이효영, 정인화

연세대 화학및의화학과

2,2-Difluoro-1-tributylstannylethenyl p-toluenesulfonate **1** was synthesized in 90% 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 tributyltin chloride. (2,2-Difluoroethene-1,1-diyl)bis(tributylstannane) **2** as an important building block was prepared in 70% yield from the reaction of 2,2-difluoro-1-tributyl-stannylethenyl p-toluenesulfonate with excess LiBr, hexabutyltin and Pd catalyst. The cross-coupling reaction **2** with 2.2 equiv of various aryl iodides in the presence of Pd and CuI catalyst afforded the symmetric 2,2-diaryl-1,1-difluoroethene **3** in 59-85% yields.



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발표분야: 유기화학

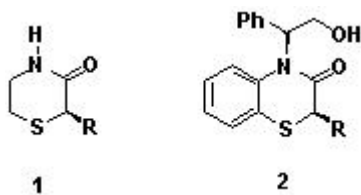
발표종류: 포스터, 발표일시: 금 15:00~17:00

## Chiral synthesis of 2-alkylidene-4-(1-phenylethyl)-3,4-dihydro-2H-benzo[b][1,4]thiazine-3(4H)-thiones

Dupati Gautam, 이은진, 신동수

창원대 화학과

Chiral 2-substituted thiomorpholin-3-one (2-STMO) **1** is a pharmacophore of great interest and derivatives containing such a sub-unit have already been prepared and evaluated in various biological fields. As one part of preparing [1,4]thiazine-3-thione scaffold, 2- substituted (R)-4-(2-hydroxy-1-phenylethyl)-2H-benzo[b][1,4]thiazin-3(4H)-one **2** were prepared by the reaction of (R)-4-(2-hydroxy-1-phenylethyl)-2H-benzo[b][1,4]thiazin-3(4H)-one via Smiles rearrangement using microwave irradiation by one-pot synthesis, followed by the reaction with alkyl halide in LDA base.



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발표분야: 유기화학

발표종류: 포스터, 발표일시: 금 15:00~17:00

## Synthesis and Characterization of a Novel Fullerene Derivative Containing Electron Rich Group for Use in Organic Solar cells

미동보, 김지훈, \*윤성철, \*\*신원석, \*\*\*이창진, 황도훈

부산대 화학과 \*한국화학연구원 화학소재연구단 \*\*한국화학연구원 에너지소재연구센터 \*\*\*한국화학연구원 화학소재연구부 소재7팀

In the quest for finding alternative solar energy generation 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, a novel fullerene derivative used as electron acceptor was synthesized via a carbene intermediate and characterized. The new synthesized fullerene derivative showed good solubility in common organic solvents and the synthetic product was characterized by  $^1\text{H}$  NMR,  $^{13}\text{C}$  NMR and FT-IR. Photovoltaic devices were fabricated using the 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. The open-circuit voltage ( $V_{oc}$ ) of the fabricated devices was found to be higher than that of devices based on  $\text{C}_{60}$  because the LUMO energy level of the new fullerene derivative was higher than that of  $\text{C}_{60}$ . Synthesis of the fullerene derivative and characteristics of the fabricated solar cells will be presented.

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장소: 제주ICC

발표코드: IV-ORGN.P-321

발표분야: 유기화학

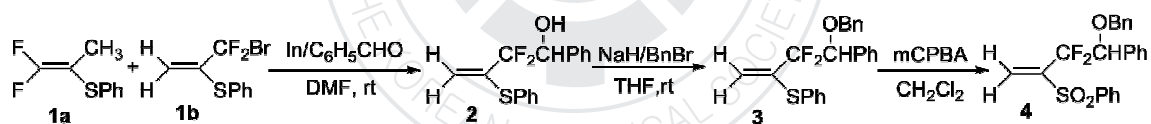
발표종류: 포스터, 발표일시: 금 15:00~17:00

## Nucleophilic addition-elimination reaction of 2-phenylsulfonyl-3,3-difluoro-4-benzyloxy-2-phenylthio-1-butene

홍윤영, 정인화

연세대 화학및의화학과

Compounds 1a and 1b were reacted with benzaldehyde in the presence of indium to give difluorohomoallylic alcohol 2. Benzylation and subsequent oxidation of 2 afforded the 4. Nucleophilic addition-elimination of 4 with alkoxide, thiolate, amine and malonate provided the corresponding vinyl fluoride as a (*E*)&(*Z*) isomeric mixture.



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발표분야: 유기화학

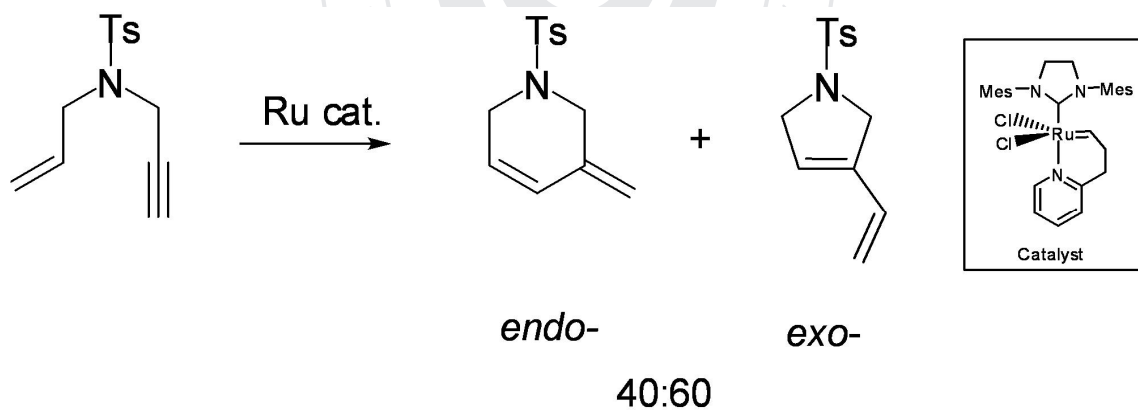
발표종류: 포스터, 발표일시: 금 15:00~17:00

## Studies on the terminal enyne ring closing metathesis

나영일, 송정아, 한소엽

이화여대 화학나노과학과, 촉매반응·합성연구센터

We studied the ring-closing metathesis (RCM) of terminal enyne using the pyridine-chelating ruthenium carbene complex. When the solution of the enyne and Ru complex in DME was refluxed under an atmosphere of Ar, both regioisomers were observed with the *endo:exo* ratio of 40:60. This work is supported by the NRF (WCU project R33-10169).



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발표분야: 유기화학

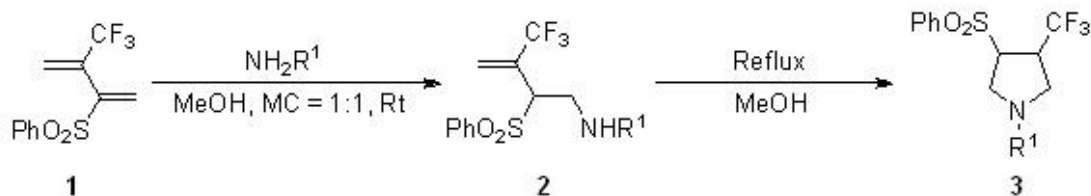
발표종류: 포스터, 발표일시: 금 15:00~17:00

## Double Nucleophilic Reactions of 2-Trifluoromethyl-3-phenylsulfonyl-1,3-butadiene

양은준, 정인화

연세대 화학및의화학과

Reaction of 2-Trifluoromethyl-3-phenylsulfonyl-1,3-butadiene **1** with primary amines provided the amine addition products **2** in good yield. The compound **2** was refluxed in MeOH to give pyrrolidine derivatives **3**. The reaction of **1** with other nucleophiles such as thiolate and alkoxide will be describes.



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발표분야: 유기화학

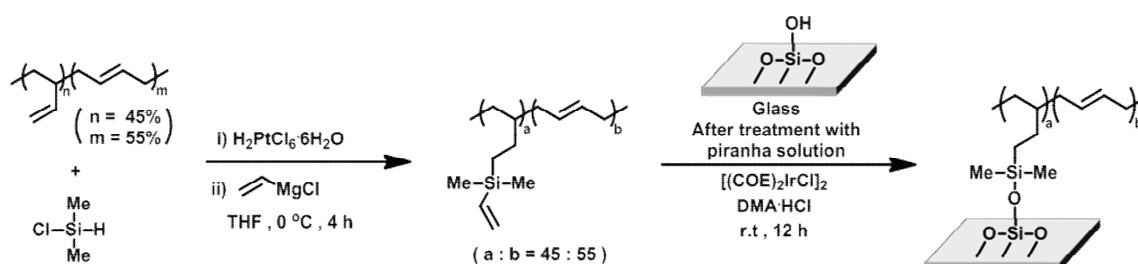
발표종류: 포스터, 발표일시: 금 15:00~17:00

## Acid-Catalyzed Immobilization of Functionalized Polybutadiene onto Solid Support

최지환, 전철호

연세대 화학과

The preparation of robust organic-inorganic hybrid material using catalyst is current interest. Recently, we developed a highly efficient immobilization method via functionalized vinylsilane under transition metal/HCl-catalytic system. Polybutadiene has many reactive terminal olefin which could be functionalized by transition metal catalyst. Synthesis of vinylsilyl group-impregnated polybutadiene was prepared by Pt-catalyzed hydrosilylation of polybutadiene with chlorodimethylsilane and treatment with vinylmagnesium chloride at 0 °C. Vinylsilyl group-impregnated polymer could be immobilized onto glass surface by Ir/HCl catalyst at room temperature. As a result, glass surface was determined as hydrophobic by contact angle measurement.



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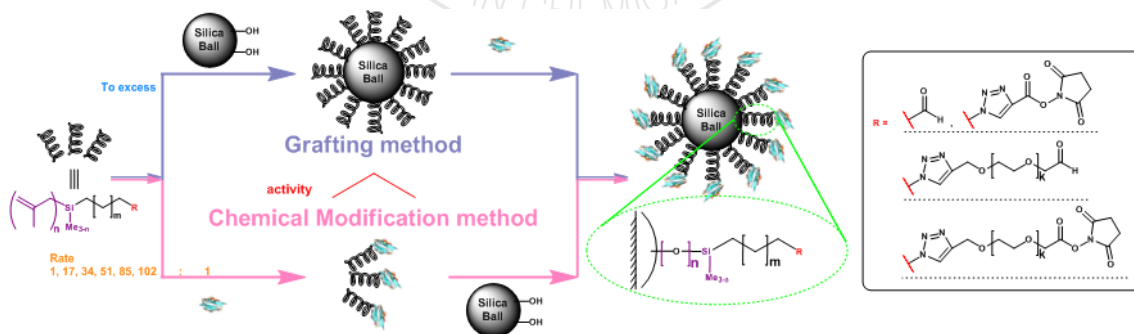
발표종류: 포스터, 발표일시: 금 15:00~17:00

## Immobilization of Enzyme: Chemical modification of Glucose Oxidase or Lipase followed by Covalent Attachment on Silica Surface

심용균, 이세라, 전철호

연세대 화학과

Methallylsilane derivative has many advantages for immobilizing organic functional group or bioactive molecules: an easiness of the specific functional group-immobilization with high efficiency under very mild condition and high loading efficiency of enzyme onto silica surface with assistance of  $\text{Sc}(\text{OTf})_3$  catalyst. In this paper, we report the immobilization of enzyme using chemical modification(CM) method. Initially enzymes were chemically modified by reacting with N-hydroxysuccinimidyl-ester or aldehyde-functionalized methallylsilane, and the resulting modified enzyme were grafted on silica surface using  $\text{Sc}(\text{OTf})_3$  catalyst at room temperature.





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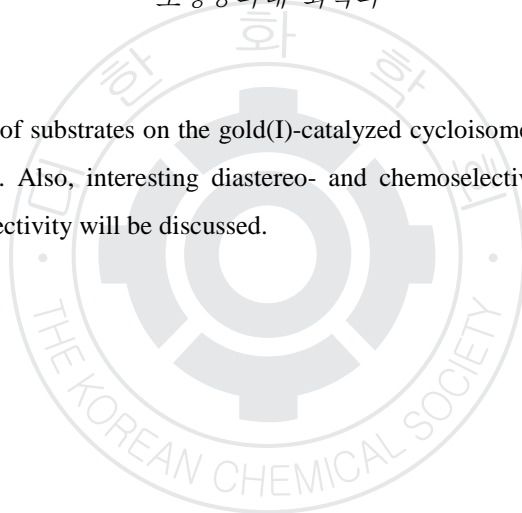
발표종류: 포스터, 발표일시: 금 15:00~17:00

## **Diastereo- And Chemoselectivity in the Gold(I)-catalyzed Cycloisomerization of Homopropargyl O,O-Acetals**

정욱, 이영호

포항공과대 화학과

Interesting structural effect of substrates on the gold(I)-catalyzed cycloisomerization of homopropargylic O,O-acetal was discovered. Also, interesting diastereo- and chemoselectivity was noted. Mechanistic rationale for this unique selectivity will be discussed.



일시: 2011년 4월 28~29일(목~금) 2일간

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발표분야: 유기화학

발표종류: 포스터, 발표일시: 금 15:00~17:00

## Synthesis and characteristics of $\alpha$ -D-glucopyranose thiol ester derivatives

김현, \*김보미, \*\*Chichong Lu, 황희민, \*\*채규윤

원광대 생명나노화학 \*원광대 생명나노 화학과 \*\*원광대 화학과

Protection of amino group of glucosamine with diethylethoxymethylene malonate followed by the reaction with acetic anhydride gave the corresponding intermediates. In this study a series of acetylated  $\alpha$ -D-glucosapyranose thiol ester were prepared using thiazolidine carboxylic acid, (ethylthio)acetic acid, (phenylthio)acetic acid, trifluoroacetic anhydride and phosphoric acid. The structural determination by FT-IR and  $^1\text{H}$  NMR was discussed. The reaction of various carboxylic acid derivatives is acetylated  $\alpha$ -D-glucopyranose thiol ester related to manufacturing methods.

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발표분야: 유기화학

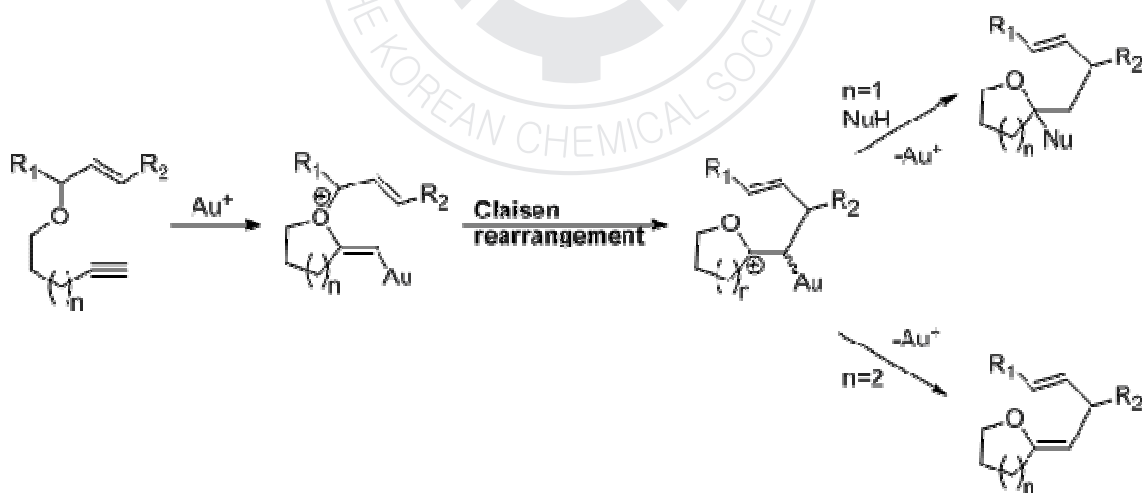
발표종류: 포스터, 발표일시: 금 15:00~17:00

## Synthesis of Tetrahydro-Furan and Pyran Derivatives in Gold(I)-Catalyzed Cyclization of n-Allyloxy-1-ynes (n = 5, 6).

정재엽, 이영호

포항공과대 화학과

Gold(I)-catalyzed reactions of 5-allyloxy-1-ynes gave tetrahydrofuran derivatives via alkoxycyclization-sigmatropic-addition sequence excluding direct demetallation[1], while the cases of 6-allyloxy-1-ynes gave tetrahydropyran derivatives which have exocyclic-double bond through direct demetallation.[1]  
Cheong, J. Y.; Im, D.; Lee, M.; Lim, W.; Rhee, Y. H. J. Org. Chem. 2011, 76, 324.



일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: IV-ORGN.P-329

발표분야: 유기화학

발표종류: 포스터, 발표일시: 금 15:00~17:00

## Synthesis and characterization of chitosan benzoates

정진아, \*Lok Ranjan Bhatt, \*송미선, \*채규윤

원광대 생명나노화학과 \*원광대 화학과

Phosphoryl mixed anhydride system was applied for the preparation of chitin benzoic acid esters. The products were characterized by  $^1\text{D}1\text{H-NMR}$  and FT-IR spectroscopy. The inclusion of benzoic acid into the resulting product was confirmed from  $^1\text{H-NMR}$  and FT-IR. The solubility of the products was tested in various organic solvents. Highest solubility was obtained when the molar ratio of trifluoroacetic anhydride, benzoic acid and phosphoric acid to chitosan was 8:4:1:1 respectively.

일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: IV-ORGN.P-330

발표분야: 유기화학

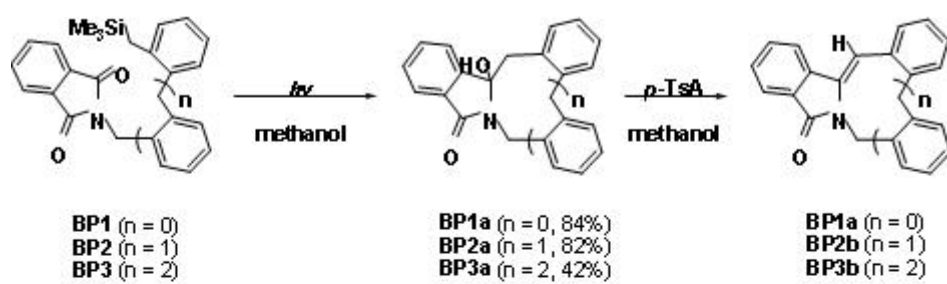
발표종류: 포스터, 발표일시: 금 15:00~17:00

## SET-Photocyclization Reactions of Silyl-Terminated Phenyl Group Containing Polydonor-Linked Phthalimides

윤기세, 안소현, 김경목, 백승진, 윤웅찬

부산대 화학과

Single electron transfer-induced photocyclization reactions of polydonor-linked phthalimides result in polyfunctionalized macrocyclic compounds. It was ether, thioether and amine chain that had been researched as electron donor in previous studies. These chains are electron-rich by reason of including oxygen, nitrogen and sulfur that have nonbonding orbitals. The photocyclization reactions of these chain-linked phthalimides produced macrocyclic products at quite high yields of 50~99%. The study on the introduction of benzene which possesses  $\pi$ -orbital and aromaticity as new electron polydonor has been carried out. Especially, target molecules for photocyclization reactions were designed to produce macrocyclic compounds more easily in molecular structure by substituting alkyl chains which link polydonor with acceptor in ortho position of benzene. Benzene was adopted for up to three and target molecules BP1~3 were synthesized. Irradiations of BP1~3 in methanol with Pyrex-filtered light resulted in the production of single non-silicon containing cyclic compounds BP1a~3a in high yields of 42~84%. Also the study on the dehydration of BP1a~3a have been researched with success. The results show that benzene can perform the function as donor in comparison with the previous studies. Furthermore, thiophene and other hetero ring aromatic compounds are expected to stand a chance as new electron donor.



일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: IV-ORGN.P-331

발표분야: 유기화학

발표종류: 포스터, 발표일시: 금 15:00~17:00

## **Efficient synthesis and characterization of benzoates chitosan derivatives**

송창현, 강경희, \*박민규, 채규윤

원광대 화학과 \*원광대 화학

Phosphoryl mixed anhydride system was applied for the preparation of chitosan benzoic acid esters. The inclusion of benzoic acid into the resulting product was confirmed from  $^1\text{H-NMR}$  and FT-IR. The solubility of the products was tested in various organic solvents. Highest solubility was obtained when the molar ratio of trifluoroacetic anhydride, benzoic acid and phosphoric acid to chitosan was 8:4:1:1. The results showed that containing benzoic acid with chitosan provides a new copolymer with improved physical properties including solubility.

일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: IV-ORGN.P-332

발표분야: 유기화학

발표종류: 포스터, 발표일시: 금 15:00~17:00

## Synthesis of Donor-Acceptor Systems Containing Benzophenone and Phthalimide as a Recyclable Photosensitizer

김성식, \*M. Sakamoto, \*T. Majima

전북대 화학과 \*Osaka University

Donor-acceptor dyads containing benzophenone and phthalimide were synthesized to investigate their photochemical properties and to find their applications. Intramolecular and intermolecular electron transfer from the benzophenone ketyl radical in the excited state to several quenchers was studied in various solvents. In addition, intramolecular triplet-triplet energy transfer from benzophenone to phthalimide was also investigated. This system was used to fabricate metal nanostructures at the solid-liquid interface. Photosensitized reduction resulted in the formation of silver nanowire or plates.



일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: IV-ORGN.P-333

발표분야: 유기화학

발표종류: 포스터, 발표일시: 금 15:00~17:00

## Thermally tunable microlenses using smectic liquid crystal defects

김정현, 정현수, 손백식, 정희태

KAIST 생명화학공학과

We demonstrate a new type of a thermally tunable microlens which is entirely based on self-assembly of liquid crystal defects. Unlike previous researches for fabricating tunable microlens using liquid crystal, this method is used solely liquid crystalline materials without mixing other materials or applying external field. Due to antagonistic anchoring conditions of liquid crystals at the smectic A and air interface in microchannels coated planar anchoring materials, smectic liquid crystals form typical defect textures called toric focal conic domains (TFCDs). TFCD-based MLAs have several advantages over other MLAs. This system focuses light using the intrinsic molecular orientations of TFCDs rather than geometrical shape, leading to high quality lens properties. Furthermore, the lens itself has tunable light transportation and all the changes could be reversibly controlled by temperature. In addition, the focal length and array number of microlens can be easily controlled by varying the feature dimension of the confined channel. Thus, this method is very easy to fabricate thermal responsive MLAs with a variety of focal length and number of array using defect structure of smectic liquid crystal.

일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: IV-ORGN.P-334

발표분야: 유기화학

발표종류: 포스터, 발표일시: 금 15:00~17:00

## Periodic spiral-shaped focal conic array using chiral smectic liquid crystal confined in microchannel

손백식, 정희태

KAIST 생명화학공학과

Production of self-assembled defect structure via aggregation of molecules is one of the key issues in advanced nanotechnologies. Use of top-down lithographic template helps not only to define size and shape of defect but also to range defect domains periodically. Recently, it has been successfully achieved to realize periodic dimple-shaped TFCD (Toric Focal Conic Domain) array by confining fluorinated smectic liquid crystal into microchannel template. Here we demonstrate highly ordered defect arrays using liquid crystals having chiral phase confined in rectangular channels. Unlike previous TFCD that is formed in SmA phase, TFCD with chiral SmC phase shows distinct spiral shape under polarized optical microscopy (POM). Movement of spiral arms of each domain has been observed under electric field. Such movement is presumed to be related to the deformed helix ferroelectric (DHF) effect caused by unwinding tendency of helical axis under electric field perpendicular to the axis. We further apply various kinds of field geometry to examine mechanism of topological deformation of TFCD.

일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: IV-ORGN.P-335

발표분야: 유기화학

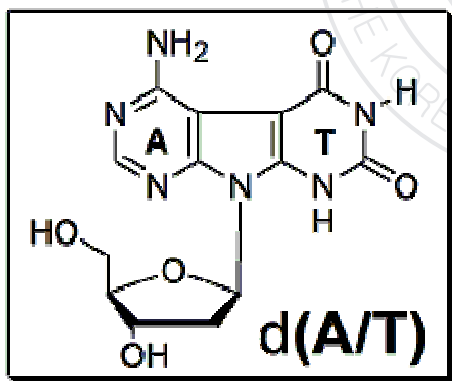
발표종류: 포스터, 발표일시: 금 15:00~17:00

## Synthesis of the nucleoside containing a dual DNA base

김경애, 황길태

경북대 화학과

We aim to design all possible nucleosides containing a dual DNA base as a new type of DNA base analogue. For the synthesis of d(A/T) which contains dA and dT simultaneously at the same molecule, we used tetracyanoethylene as starting material. As a key reaction, we got the  $\beta$ -anomer in high yield via glycosylation reaction with sodium hydride. Synthetic details, and fluorescence properties of a dual nucleobase will be discussed.



일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: IV-ORGN.P-336

발표분야: 유기화학

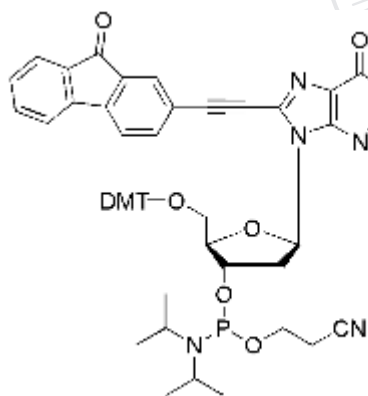
발표종류: 포스터, 발표일시: 금 15:00~17:00

## Fluorenone-labeled deoxyguanosine: Synthesis and Its fluorescence properties upon duplex formation

서유진, 황길태

경북대 화학과

We developed a fluorenone-labeled deoxyguanosine ( $G^{FO}$ ) unit as a new fluorescence probe. We analyzed its fluorescence change upon duplex formation with its complementary matched- and mismatched sequences. Additionally, the effect of DNA length, sequences, direction, and 3D structure on the oxidative DNA damages induced by photo-irradiation will be described.



일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: IV-ORGN.P-337

발표분야: 유기화학

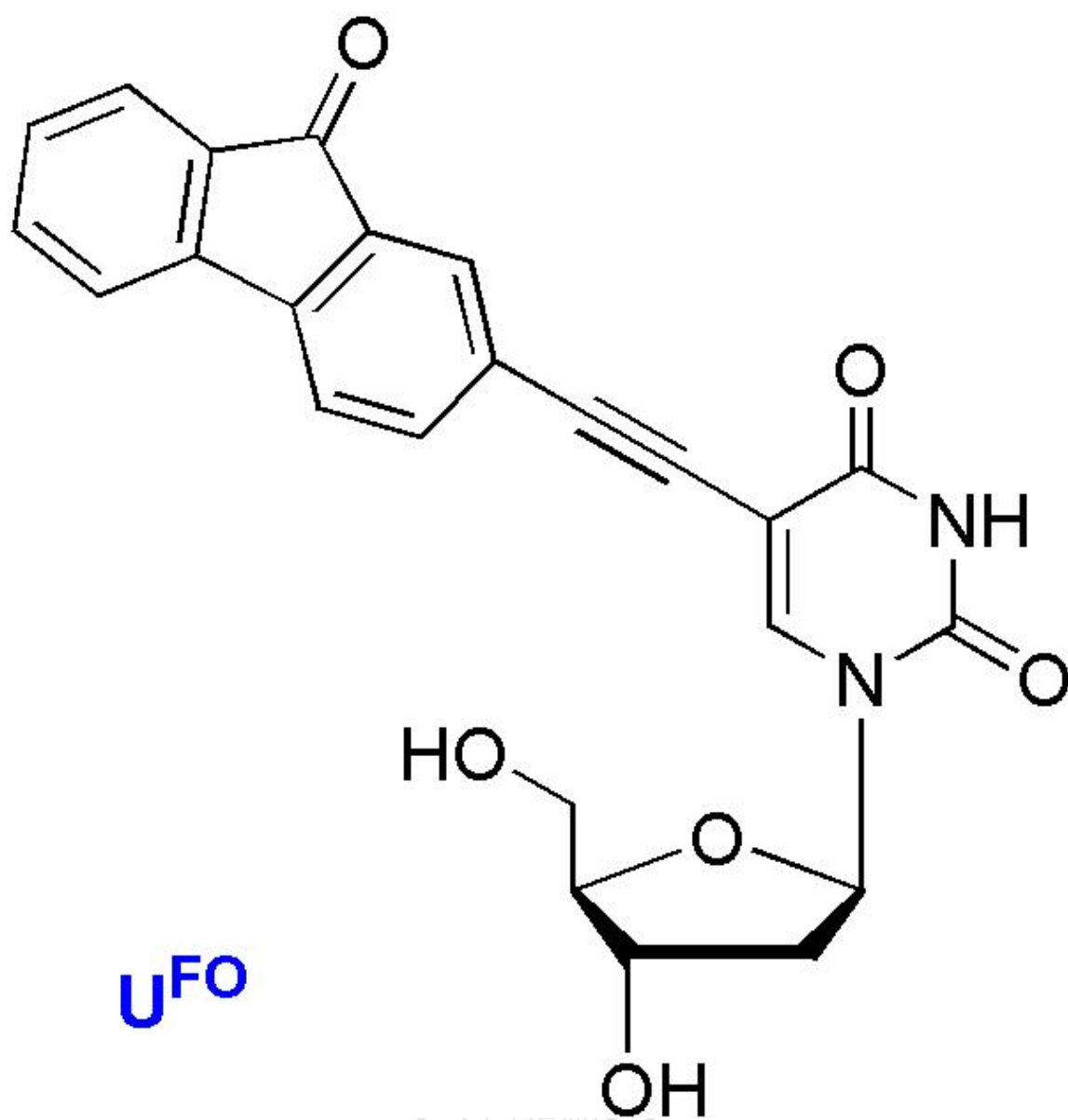
발표종류: 포스터, 발표일시: 금 15:00~17:00

## Sequence-specific fluorescence changes of DNA containing 5-(2-ethynyl-9-fluorenone)-2'-deoxyuridine

허주영, 황길태

경북대 화학과

To investigate the behavior of fluorescence intensity, we designed an dA-selective fluorescent DNA probe ( $U^{FO}$ ), at which 2-ethynyl-9-fluorenone moiety is covalently attached, and incorporated it in the linear single-stranded beacon probe. The fluorescence of  $U^{FO}$  displayed a strong dependence on the nature of its flanking bases (FBs). When the FBs were T or C, it exhibited high total discrimination factors for the formation of perfectly matched- and single base mismatched duplexes. We will describe photophysical properties of the  $U^{FO}$  DNA probe and its application to single-nucleotide polymorphism (SNP) typing.



U<sup>FO</sup>

일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: IV-ORGN.P-338

발표분야: 유기화학

발표종류: 포스터, 발표일시: 금 15:00~17:00

## Synthesis of 2,6-Diaryldiphenyldithienosilole Derivatives and Its application in OLED

곽영우

경북대 화학과

The dithienosilole derivatives (DTS-TAZ and DTS-OXD) containing para-substituted phenyl with triazole and oxadiazole groups connected to the bithiophene moiety of the DTS were successfully synthesized by Pd(PPh<sub>3</sub>)<sub>4</sub>-catalyzed Suzuki cross coupling reactions. The UV-vis absorption and emission maxima, TGA, DSC, and Oxidation potential of these new derivatives were measured. For the evaluation of the electroluminescent properties [current density-voltage, luminance-voltage, efficiency(lm/W)-luminance(cd/m<sup>2</sup>), CIE(x,y), and EL spectra of DTS-TAZ and DTS-OXD derivatives], these derivatives were used as electron-transporting layers in electroluminescent(EL) device fabrication processes. The device structures were ITO/LHT001(600 Å)/LHT211(300 Å)/LBH009 : BD052X(300 Å) : 7%)/ETL(200 Å)/LiF/Al.

일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: IV-ORGN.P-339

발표분야: 유기화학

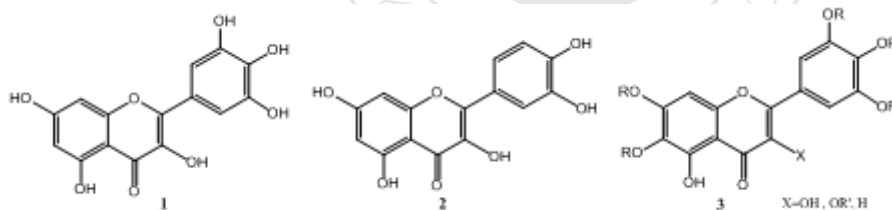
발표종류: 포스터, 발표일시: 금 15:00~17:00

## Synthesis Of Relatively Hydrophobic 3-deoxy-Myricetin Derivatives As A Potent SNARE-protein Inhibitor

고미선, 박훈규, 김보정,\*이강우, 김학원

경희대 화학과 \*경희대 응용화학과

기존 연구결과에 의하면 자연계에 존재하는 flavonoids 화합물중에서 Myricetin(1)과 Quercetin(2)가 높은 SNARE-dependent Neuroexocytosis 에 활성을 보인다고 보고되어 있다. 따라서, 본 연구에서는 Myricetin 과 유사한 구조의 유도체들(3), 특히 보다 hydrophobic 하고 3 위치에 hydroxy 기가 있거나, 없는 유도체들을 설계, 합성하는 방법을 연구하였으며, 합성된 유도체들의 biological activity 를 조사하였다.





일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: IV-ORGN.P-340

발표분야: 유기화학

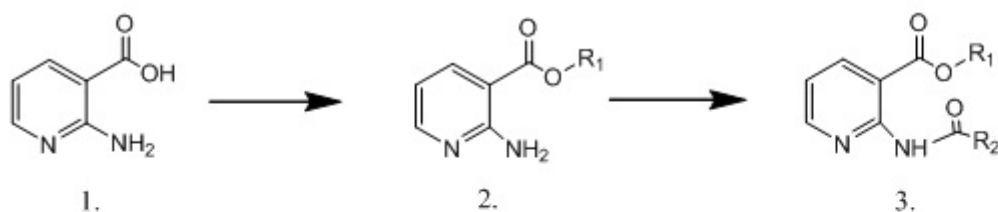
발표종류: 포스터, 발표일시: 금 15:00~17:00

## Synthesis and Evaluation of N-acyl-2-aminonicotinate as a CO<sub>2</sub>-philic Chelating Ligand

권현지, 임병조, 김학원

경희대 화학과

본 발표에서는 Supercritical-CO<sub>2</sub> 상에서 금속을 추출할 수 있는 친이산화탄소성킬레이트 리간드 개발과 관련한 연구결과를 보고하고자 한다. 본 연구에서는 2-Aminonicotinic acid(1)를 esterification 을 통해 ester 유도체(2)를 합성하였고, N-acylation 을 통해 N-acylated 2-Aminonicotinate(3)를 친이산화탄소성 킬레이트 리간드로 합성하여, 이들 유도체들의 초임계이산화탄소에서의 용해도와 금속이온 추출정도를 조사하였다.



일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: IV-ORGN.P-341

발표분야: 유기화학

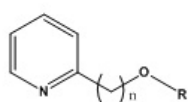
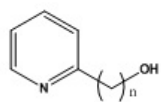
발표종류: 포스터, 발표일시: 금 15:00~17:00

## Synthesis of CO<sub>2</sub>-philic 2-substituted pyridine derivatives and metal extraction in sc-CO<sub>2</sub>

임병조, 노경탁, 김학원

경희대 화학과

본 발표에서는 Supercritical-CO<sub>2</sub> 상에서 금속을 추출할 수 있는 친이산화탄소성 킬레이트 리간드 개발과 관련한 연구결과를 보고하고자 한다. 2 위치가 hydroxy alkyl 기로 치환된 pyridine(2-pyridinemethanol, 2-pyridineethanol)화합물의 hydroxy group 에 여러 가지 carbonyl group 과 ether group 을 도입하여 다양한 2-pyridinealkyl ester 및 ether 유도체들을 합성하였고, 이의 CO<sub>2</sub>-solubility 를 측정, 비교하였고, 이를 이용하여 초임계이산화탄소에서 금속이온을 추출하는 연구를 수행하였다.



일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: III-MEDLP-205

발표분야: 의약화학

발표종류: 포스터, 발표일시: 금 10:30~12:30

## Development of Isozyme Selectivity Model for Phase II Metabolism Using SVM Method

강신문, \*오원석, \*\*김선영, \*\*\*남기엽, \*노경태

(사)분자설계연구소 신약개발 \*연세대 생명공학과 \*\*분자설계연구소 신약개발팀 \*\*\* (사)분자설계연구소 신약개발실

Developing effective tools for predicting absorption, distribution, metabolism, excretion properties and toxicity (ADME/T) of new chemical entities in the early stage of drug design is one of the most important tasks in drug discovery and development today. Drug-Metabolism, one of ADME properties, is important property including metabolite stabilization, drug-drug interaction and drug toxicity. The metabolism of xenobiotics is often divided into three phases: Phase I - modification, Phase II - conjugation, and Phase III - excretion. These reactions act in concert to detoxify xenobiotics and remove them from cells. In general, conjugation with phase II drug metabolizing enzymes(DMEs) generally increases hydrophilicity, and thereby enhance excretion in the bile and/or the urine and consequently a detoxification effect. Although under certain situations, conjugation with phase II enzymes could result in activated metabolites and increase toxicity. In this account, we are interested in 4 metabolism reaction of phase II, Glucuronidation(UGT), Sulfation(SULT), Acetylation(NAT) and Glutathione conjugation(GST). Support Vector Machines (SVM) has recently been exploited for the prediction of ADME/T related properties. However, two problems in SVM modeling, i.e. feature selection and parameters optimization, are still far from being solved. The two problems have been shown to be crucial to the efficiency and accuracy of SVM classification. In particular, several solutions have been suggested for feature selection such as genetic algorithm(GA), recursive feature eliminations(RFE), simulated annealing approach(SA), and so on. In these methods, we were able to cut calculation time using genetic algorithm(GA) for parameters optimization. So we tried to improve accuracy of drug-metabolizing enzymes prediction models using GA-GA-SVM

일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: III-MEDLP-206

발표분야: 의약화학

발표종류: 포스터, 발표일시: 금 10:30~12:30

## Computational Drug Discovery Approach Based on Nuclear Factor- $\kappa$ B Pathway Dynamics

김선영, \*오원석, \*\*강신문, \*\*\*남기엽, \*노경태

분자설계연구소 신약개발팀 \*연세대 생명공학과 \*\* (사)분자설계연구소 신약개발 \*\*\* (사)분자설계연구소 신약개발실

The NF- $\kappa$ B system of transcription factors plays a crucial role in inflammatory diseases. In order to cure inflammatory related diseases, Many compounds can were identified as IKK $\beta$  inhibitors with high-throughput screening and virtual screening. We combine quantitative structure activity relationship for predicting the activity of new compounds and quantitative dynamic model for the NF- $\kappa$ B network with intracellular concentration models. We employed GFA-MLR QSAR analysis to search for the optimal QSAR equation. To validate the predictability of the IKK $\beta$  QSAR model on external set of inhibitors, We modelled NF- $\kappa$ B dynamic system using a set of ordinary differential equation and mass action kinetics. The reaction parameters were obtained from Hoffmann's paper. In the IKK $\beta$  QSAR model, Good cross-validated  $q^2$ (0.782) and conventional  $r^2$ (0.808) values proved the correlation between the descriptors and each of their activities, and gave reliability to the prediction of the IKK $\beta$  activities. We have developed a simulation model of NF- $\kappa$ B signal pathway with quantitative information of reaction rate and the molecular concentration of signaling entities.

일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: III-MEDLP-207

발표분야: 의약화학

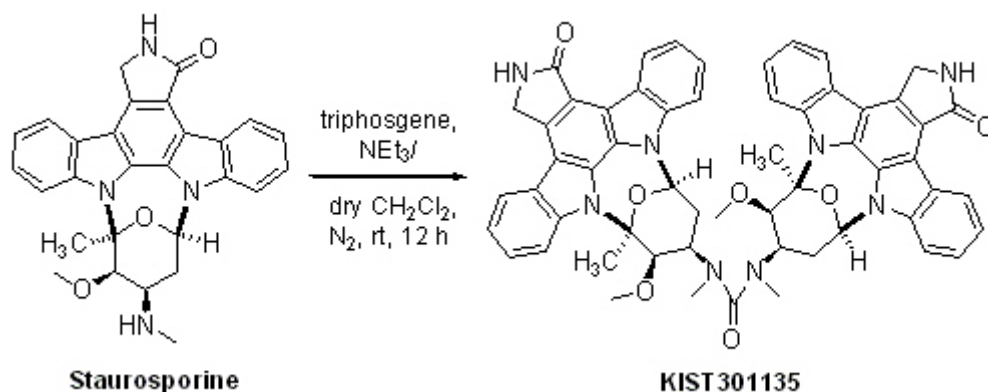
발표종류: 포스터, 발표일시: 금 10:30~12:30

## Synthesis of Staurosporine dimer and its selective anticancer activity

정수진, \*Ibrahim M. El-Deeb, \*\*최기향, \*\*\*이소하

고려대 \*Griffith University \*\*고려대 화학과 \*\*\*KIST 바이오소재연구센터

The high structural conservation of kinases causes selectivity problems in most drug inhibitors, often resulting in dangerous side effects. This is often the reason behind the failure of many kinase inhibitors in the clinical trials. The selectivity of such inhibitors could be however improved by the use of selectivity filters (unique structural features in the intended target that are liable for discrimination by a rationally designed inhibitor). In this study, a new highly selective Staurosporine derivative, KIST301135 has been designed, synthesized and screened over a panel of 53 kinases against Staurosporine as a control compound. The new inhibitor, KIST301135, has showed much improved kinase inhibitory selectivity relative to Staurosporine, without a significant decrease in potency, with marked activity over JAK3 and CAMK2b kinases. The new compound was designed using a new selectivity filter that utilizes the differences in binding pockets geometry in different kinases as a filtration tool. This new approach of "size exclusion" provides a new simple and efficient method for the re-design of a large number of potent but non-selective kinase inhibitors already available, in order to qualify them to be employed as more selective inhibitors in different treatments.



일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: III-MEDLP-208

발표분야: 의약화학

발표종류: 포스터, 발표일시: 금 10:30~12:30

## Synthesis and Biological Evaluation of New Arylpiperazine-Containing Imidazole 4-Carboxamide Derivatives: Targeting 5-HT<sub>2A/2C</sub> Receptor Antagonist and the Serotonin Reuptake Inhibitor as a Potential Antidepressant

서희정, 박은정, 이석호, 김정민, 이진화

(주)녹십자

Serotonin antagonist/reuptake inhibitor (SARI) drugs that block both the serotonin 5-HT<sub>2</sub> receptors and the serotonin transporters have been developed. The human 5-HT<sub>2A/2C</sub> receptor has been implicated in several neurological conditions, and potent and selective 5-HT<sub>2A/2C</sub> ligands may have therapeutic potential for treatment of CNS diseases, such as depression. Therefore, the receptors have been considered as reasonable targets for the improved treatment of depression. An imidazole moiety usually provides good pharmacokinetic properties as a drug substance and thus considerable efforts have been devoted to develop imidazole derivatives into drug candidates. The imidazole library was evaluated against serotonin receptors (5-HT<sub>2A/2C</sub>) and serotonin reuptake inhibition. Some of the compounds show promising IC<sub>50</sub> values and antidepressant-like effect in *in vivo* forced swimming test (FST). Based on these results, further lead optimization studies resulted in more potent compound.

일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: III-MEDLP-209

발표분야: 의약화학

발표종류: 포스터, 발표일시: 금 10:30~12:30

## Isolation and identification of three flavonoids from *Allium Mongolicum*

tuvaagerel, 이범중

인제대 화학과

*Allium Mongolicum* is an endemic native plant in Mongolia. In tradition of Mongolia, this plant has been used for food such as onion. There is no information about the isolation of any bioactive secondary metabolites from this plant. The purpose of our study is to isolate bioactive compounds from *Allium Mongolicum*. We isolated three bioactive flavonoids from ethyl acetate fraction of *Allium Mongolicum*, which shows anti-oxidant and cytotoxicity activity. We analysed the anti-oxidant and cytotoxicity activity of these compounds by some in-vitro assay methods. The structure of compounds has been elucidated by combined spectroscopic methods including  $^{13}\text{C}$  and  $^1\text{H}$ -NMR, LC-MS, IR and UV-Vis.



일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: III-MEDLP-210

발표분야: 의약화학

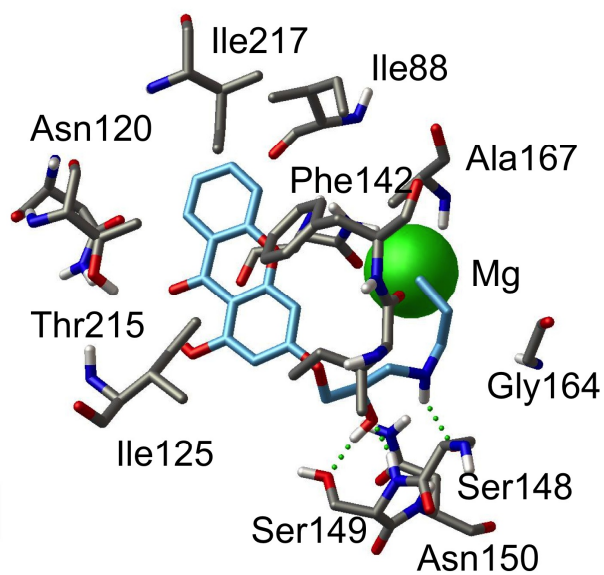
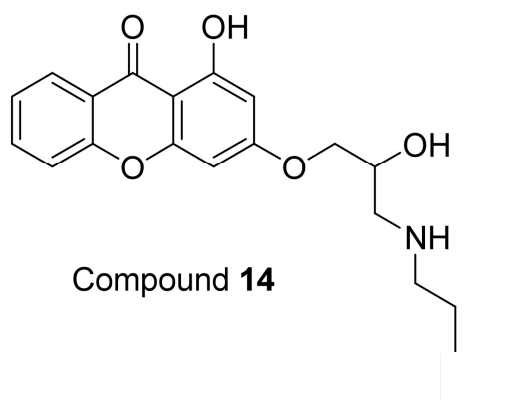
발표종류: 포스터, 발표일시: 금 10:30~12:30

## **Molecular docking study of 3-(3'-heteroatom substituted-2'-hydroxy-1'-propyloxy) xanthone analogues as novel topoisomerase II $\alpha$ catalytic inhibitor**

전규연

이화여대 약학대학

Eight novel heteroatom nucleophilic epoxide ring-opened xanthone derivatives were designed and synthesized for the development of topoisomerase II $\alpha$  (topo II $\alpha$ ) inhibitors. These compounds were first tested for their topoisomerase inhibitory activity and cytotoxicity. Most of the compounds showed topo II $\alpha$  specific inhibitory activity. To clarify the mechanism of action of these compounds, the most potent compound (compound 14) of the synthesized analogues was further studied by testing its ATPase inhibitory activity and through molecular docking experiments. The results showed that the topo II $\alpha$  inhibitory activity of compound 14 was inversely proportional to ATP concentration. In the ATPase inhibitory test, ATP hydrolysis was reduced less efficiently by compound 14 ( $28.5 \pm 4.6$  %) than novobiocin ( $60.4 \pm 8.1$  %). The molecular docking study revealed compound 14 to have a stable binding pattern to the ATP-binding domain of human topo II. Overall, compound 14 can be a novel scaffold as a human topo II $\alpha$  specific inhibitor focusing on its ATP-binding domain.



일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: III-MEDLP-211

발표분야: 의약화학

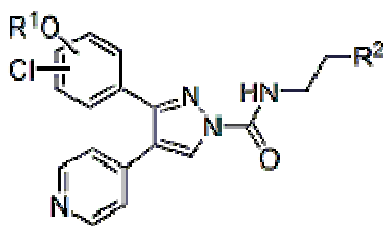
발표종류: 포스터, 발표일시: 금 10:30~12:30

## New 3,4-diarylpyrazole-1-carboxamide derivatives: Design, synthesis, and anticancer evaluation

**Mohammed I. El-Gamal**, \*이웅산, \*\*유경호, \*\*조정혁, \*\*\*오창현

과학기술연합대학원대 Medicinal Chemistry \*고려대 화학과 \*\*KIST 생체과학연구본부 \*\*\*KIST  
바이오소재연구센터

Design and synthesis of a new series of 3,4-diarylpyrazole-1-carboxamide derivatives are described. Their antiproliferative activity against A375 human melanoma cell line was tested and the effect of substituents on the diarylpyrazole scaffold was investigated. In addition, 29 target compounds were tested at a single dose concentration of 10  $\mu$ M over a panel of 60 cancer cell lines of 9 different cancer types at the National Cancer Institute (NCI), Bethesda, Maryland, USA. Among these 29 compounds, 4 were selected for 5-dose testing in order to determine their IC<sub>50</sub>, TGI, and LC<sub>50</sub> values over the 60 cell lines. These 4 tested derivatives showed high potency and efficacy against most of the 60 cell lines.



R<sup>1</sup> = H, CH<sub>3</sub>

R<sup>2</sup> = dialkylamino, heterocycloalkyls

일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: III-MEDLP-212

발표분야: 의약화학

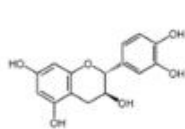
발표종류: 포스터, 발표일시: 금 10:30~12:30

## Tyrosinase and elastase inhibitory constituents from the stems of *Neolitsea aciculata*

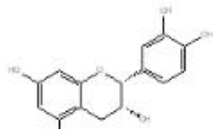
김상숙, 이남호

제주대 화학과

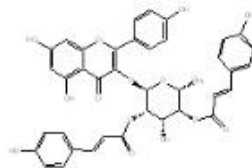
Bioassay-guided investigation of the stems of *Neolitsea aciculata* led to the isolation of 10 compounds: catechin (1), epicatechin (2), kaempferol 3-O- $\alpha$ -L-(2'',3''-E-di-p-coumaroyl)-rhamnoside (3), 2''-p-coumaroylafzelin (4), feruloyl tyramine (5), aralia cerebroside (6),  $\beta$ -sitosterol (7), daucosterol (8), oleic acid (9), and trilaurin (10). Their structures were elucidated on the basis of spectroscopic studies as well as by comparison with available data in the literature. Among these isolates, compounds 3, 4, and 6 were identified as potent tyrosinase inhibitors. It inhibited mushroom tyrosinase with IC<sub>50</sub> values of 49.11, 46.76, and 31.74  $\mu$ g/mL, respectively. The inhibition kinetics, analysed by Lineweaver-Burk plots, indicated compounds 3 and 4 to be competitive inhibitors of tyrosinase when L-tyrosine was used as a substrate. Compounds 3, 4, and 5 showed significant elastase inhibition activities and IC<sub>50</sub> values were 26.2, 77.3, and 62.4  $\mu$ g/mL, respectively. Interestingly, compounds 1-10 were isolated for the first time from this plant.



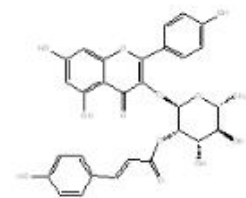
Catechin (1)



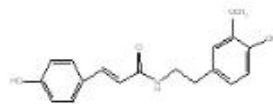
*epi*-catechin (2)



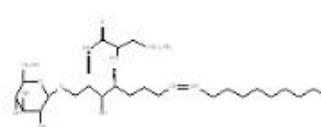
Kaempferol 3-O- $\alpha$ -L-(2'',3''-E-di-*p*-coumaroyl)-rhamnoside (3)



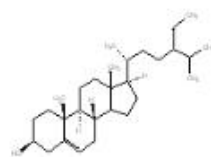
2''-*p*-coumarolyafzelin(4)



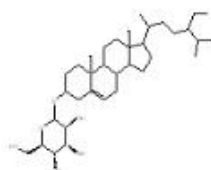
Feruloyl tyramine(5)



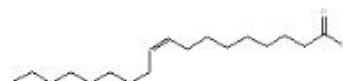
Aralia cerebroside (6)



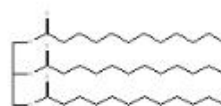
$\beta$ -sitosterol (7)



Daucosterol (8)



Oleic acid (9)



Trilaurin (10)



일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: III-MEDLP-213

발표분야: 의약화학

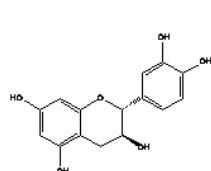
발표종류: 포스터, 발표일시: 금 10:30~12:30

## Flavonoids with Antioxidative Activities from *Cleyera japonica* Thunb

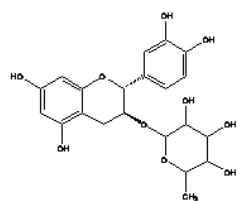
김정은, 정덕상, 이남호

제주대 화학과

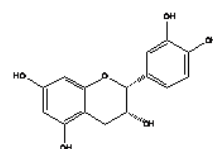
Phytochemical investigation of the ethanol extract from *Cleyera japonica* Thunb. stem resulted in the isolation of seven flavonoids; catechin (1), catechin 3-*O*- $\alpha$ -L-rhamnopyranoside (2), *epi*-catechin (3), taxifolin (4), taxifolin 3-*O*- $\alpha$ -L-arabinopyranoside (5), taxifolin 3-*O*- $\alpha$ -L-rhamnopyranoside (6), proanthocyanidin A-1 (7). The 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 1-7 were isolated for the first time from this plant. DPPH and hydroxyl radical scavenging activities were investigated for the isolated compounds. All of the compounds showed strong DPPH radical scavenging activities with  $SC_{50}$  of 5.0  $\mu$ g/mL (1), 10.0  $\mu$ g/mL (2), 6.6  $\mu$ g/mL (3), 6.3  $\mu$ g/mL (4), 13.2  $\mu$ g/mL (5), 8.6  $\mu$ g/mL (6) and 5.4  $\mu$ g/mL (7) respectively, whose activities were comparable to a positive control vitamin C ( $SC_{50}$  4.1  $\mu$ g/mL). In addition, compounds 1, 3, 4 and 7 showed strong hydroxyl radical scavenging activities with  $SC_{50}$  of 614.9  $\mu$ g/mL (1), 625.4  $\mu$ g/mL (3), 395.8  $\mu$ g/mL (4) and 173.9  $\mu$ g/mL (7) respectively, where the activity of vitamin C was  $SC_{50}$  151.4  $\mu$ g/mL. Based on these results, *C. japonica* stem extract could be potentially applicable as antioxidant.



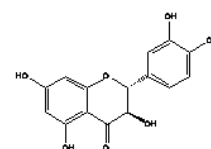
Catechin  
(compound 1)



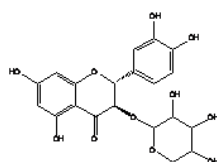
Catechin 3-O-α-L-rhamnopyranoside  
(compound 2)



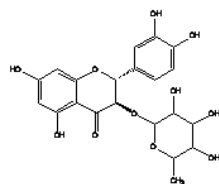
epi-catechin  
(compound 3)



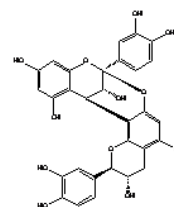
Taxifolin  
(compound 4)



Taxifolin 3-O-α-L-arabinopyranoside  
(compound 5)



Taxifolin 3-O-α-L-rhamnopyranoside  
(Astilbin) (compound 6)



epi-catechin-(2β→O→7, 4β→8)-catechin  
(Proanthocyanidin A-1) (compound 7)



일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: III-MEDLP-214

발표분야: 의약화학

발표종류: 포스터, 발표일시: 금 10:30~12:30

## Design of D-ring removed Estradiol Analogues as SERMs

이선영, \*김희두, \*\*장일명

숙명여대 약학과 \*숙명여대 약학대학 \*\*숙명여대 제약학과

Estrogens play a central role in female reproduction and exert beneficial effects on the skeletal, cardiovascular, and central nervous systems. In clinical observations, postmenopausal women have a higher incidence of osteoporotic fractures, coronary heart disease, hot flashes, and night sweats and a lower reported quality of life. There remains a role in women's health for Hormone replacement therapy(HRT), however, the place of the current agents, based upon conjugated equine estrogens, may be filled by selective estrogen receptor modulators (SERMs), particularly for women at high risk of breast cancer. The first, second generation SERMs have a side effect. So we aimed at the discovery of a new class of next generation SERMs, endowed with pharmacological profiles acting as agonists for bone system and as antagonists for cancers for the treatment of osteoporosis and estrogen-responsive breast cancer. And we have focused on similar approach for estradiol derivatives and structural modifications was carried out the synthesis of new scaffold SERMs. The D-ring removed 17  $\beta$ -estradiol analogues as SERMs were designed, synthesized and evaluated their affinity with ER. We are synthesizing D-ring removed estradiol analogues to evaluate the better affinity and the tissue selective action of SERM.



일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: III-MEDLP-215

발표분야: 의약화학

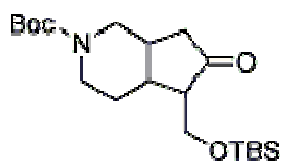
발표종류: 포스터, 발표일시: 금 10:30~12:30

## Synthesis of a hexahydro-cyclopenta[c]pyridine ring as a novel scaffold for GPCR modulators

최정환, 하덕찬, \*박철민, \*\*이선경

고려대 화학과 \*한국화학연구원 의약화학 연구센터 \*\*한국화학연구원 의약화학연구센터

This presentation will discuss the synthetic method of a hexahydro-cyclopenta[c]pyridine ring as a novel scaffold of drug candidates, especially GPCR modulators. The [6+5] fused bicycle was efficiently prepared by intramolecular Pauson-Khand reaction using dicobalt octacarbonyl. The terminal alkyne, a key intermediate, was prepared starting from 2,2-diethoxypropane-1-amine through the series of reactions including the protection of amine, deprotection of an acetal to aldehyde, Wittig reaction to give an  $\alpha,\beta$ -unsaturated ester, reduction of an ester to alcohol, protection of an alcohol, alkylation of the protected amine with propargyl halide.



일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: III-MEDLP-216

발표분야: 의약화학

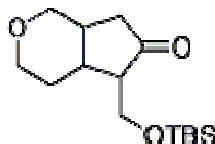
발표종류: 포스터, 발표일시: 금 10:30~12:30

## Synthesis of a octahydro-cyclopenta[c]pyran ring as a novel scaffold for GPCR modulators

최정환, 하덕찬, \*박철민, \*\*이선경

고려대 화학과 \*한국화학연구원 의약화학 연구센터 \*\*한국화학연구원 의약화학연구센터

The octahydro-cyclopenta[c]pyran ring as a novel scaffold of drug candidates, especially GPCR modulators was prepared efficiently using intramolecular Pauson-Khand reaction as a key step. The starting material, 1,4-propane diol was mono-alkylated using propargyl halide, and the remaining alcohol was reduced to aldehyde, which was converted to an  $\alpha,\beta$ -unsaturated ester by Wittig reaction. The ester was reduced to an alcohol, following the protection. The intramolecular cycloaddition of an alkene, alkyne using dicobalt octacarbonyl provided [6+5] fused bicycle, and the double bond was subsequently reduced by hydrogenation.



일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: III-MEDLP-217

발표분야: 의약화학

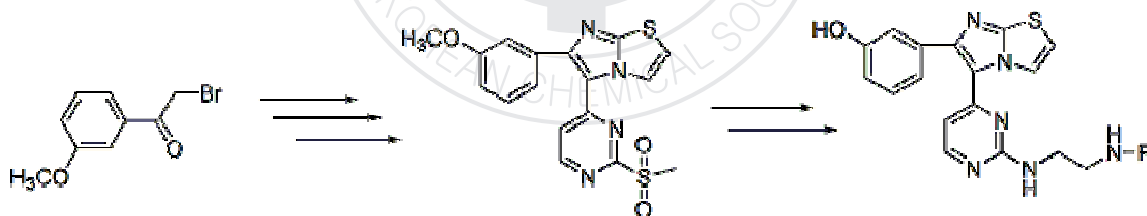
발표종류: 포스터, 발표일시: 금 10:30~12:30

## Synthesis of imidazo[2,1-b][1,3]thiazole derivatives and their antiproliferative activity against melanoma cell line

이용산, \*Mohammed I. El-Gamal, \*\*심태보, \*\*유경호, \*\*조정혁, \*\*\*오창현

고려대 화학과 \*과학기술연합대학원대 Medicinal Chemistry \*\*KIST 생체과학연구본부 \*\*\*KIST  
바이오소재연구센터

Melanoma is the most aggressive form of skin cancer and is the fastest growing cancer in the United States. In this study, synthesis of a new series of imidazo[2,1-b][1,3]thiazole derivatives is described. Their in vitro antiproliferative activity against A375 human melanoma cell line and structure-activity relationship (SAR) study are reported.



일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: III-MEDLP-218

발표분야: 의약화학

발표종류: 포스터, 발표일시: 금 10:30~12:30

## Development of *in silico* Metabolic Stability with Phase I Metabolism Prediction

정승화, \*남기엽, 노경태, 오원석

연세대 생명공학과 \* (사)분자설계연구소 신약개발실

Metabolic stability is an important property of drug candidates. Most of the drug metabolism occurs by cytochrome P450 isoenzymes, the accurate prediction of CYP450-mediated metabolic reactions is necessary for efficient drug discovery. The EaMEAD method previously described enables early prediction of the regioselectivity of metabolic reactions in a practical and efficient manner. We developed the simulation method of first-order reaction kinetics for the quantitative drug metabolism reaction of CYP450 3A4. The predicted drug metabolic stabilities were compared with the experimental % remaining of drug after 30min. The reliability and ease of use of this model will greatly facilitate early stage PK predictions and rational drug design

일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: III-MEDLP-219

발표분야: 의약화학

발표종류: 포스터, 발표일시: 금 10:30~12:30

## The Validation of docking tools for PAK4 Drug Discovery

정명기, 노경태, \*남기엽

연세대 생명공학과 \*(사)분자설계연구소 신약개발실

The Rho-family GTPases Rho, Rac and Cdc42 regulate many intracellular processes through their interaction with downstream effector proteins. The PAKs (p21-activated kinases) are a family of effector proteins for Rac and Cdc42. The PAKs are important regulators of actin cytoskeletal dynamics, neurite outgrowth, cell survival, hormone signaling and gene transcription. A PAK4 is the only PAK-family member that is oncogenic when overexpressed and promotes tumorigenesis in vivo. Our goal is discovering therapeutic potential PAK4 inhibitors using structure based virtual screening technique. Before virtual screening, we have validated a docking tool like Autodock and LigandFit. We compared the correct binding results with two x-ray crystal PAK4 inhibitors with Autodock rigid docking, flexible docking and LigandFit. We performed the cross docking with five x-ray crystal PAK4 structures and two known inhibitors using each docking method. The results show that the rigid docking methods provide prominent performance in self docking and the flexible docking exhibits the improved performance in cross docking. These results have to apply for virtual screening.

일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: III-MEDLP-220

발표분야: 의약화학

발표종류: 포스터, 발표일시: 금 10:30~12:30

## Synthesis and characterization of gold nanoparticles based on water-soluble Purpurin-18-N-methyl-D-glucamine.

Lkhagvadulam, 김정화, \*윤일, \*\*심영기

인제대 나노시스템공학과 \*인제대 PDT 연구소 \*\*인제대 나노공학부

We have synthesized a new type of water soluble ionic photosensitizer Purpurin-18-N-methyl D-glucamine. And it was transformed into a small gold nanoparticles stabilized by the photosensitizer without adding any particular reducing agents and surfactants. UV-Vis spectroscopy, Transmission Electron Microscopy (TEM), dynamic light scattering (DLS), TGA, XRD, ATR-IR, <sup>1</sup>H-NMR, EA, MS were used to confirm the formation of gold nanoparticles and photosensitizer. PDT Research Institute, School of Nano Engineering Systems, Inje University, Gimhae, KOREA, Correspondence to Y. K. Shim: (ykshim@inje.ac.kr)

일시: 2011년 4월 28~29일(목~금) 2일간

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발표코드: III-MEDLP-221

발표분야: 의약화학

발표종류: 포스터, 발표일시: 금 10:30~12:30

## **Cyclophilin D inhibitors to block Ab-mediated mPTP formation for Alzheimer's disease**

김지윤, \*추현아, 문봉진

서강대 화학과 \*KIST 생체과학연구부

Amyloid beta(A $\beta$ ) plays a critical role in the pathophysiology of Alzheimer's disease. However, the effects of A $\beta$  toxicity on mitochondria have not yet been fully elucidated. Recent biochemical studies have implicated the involvement of mitochondrial permeability transition pore (mPTP) formation in A $\beta$ -mediated mitochondrial dysfunction. mPTP is composed of ANT in the inner mitochondrial membrane, VDAC of the outer membrane, and the matrix protein CypD (cyclophilin D). Recently, it was reported that cyclosporin A (CsA), known as inhibitor of CypD, effectively inhibited mPTP formation mediated by Ab, resulting in protecting mitochondria. Therefore, CypD is a very important molecular target for treatment of Alzheimer's disease. There have been few inhibitors of CypD discovered. To find new inhibitors of CypD, known inhibitors of CypA with more than 90% similarity to CypD were modified and the modified compounds were synthesized and biologically evaluated against A $\beta$ -mediated mitochondrial dysfunction. The synthesis and biological activity will be discussed in detail.

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발표종류: 포스터, 발표일시: 금 10:30~12:30

## 2-Methoxypiperazine derivatives as 5-HT7 receptor antagonists

김영재, \*추현아

과학기술연합대학원대 의약및약품화학 \*KIST 생체과학연구부

5-HT7 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-HT7 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-HT7 receptor is engaged in the pathomechanism of depression. Thus, 5-HT7 receptor is potentially a good target for treatment of depression. Based on the known 5-HT7 receptor ligands, 2-methoxypiperazine derivatives was designed, synthesized and biologically evaluated against 5-HT7 receptor. The synthesis and biological activity will be discussed in detail.



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발표종류: 포스터, 발표일시: 금 10:30~12:30

**Synthesis and characterization of gold nanoparticles based on water-soluble chlorin-p6 6-Ne-lysylamide -7- methyl ester.Synthesis and characterization of gold nanoparticles based on water-soluble chlorin-p6 6-Ne-lysylamide -7- methyl ester.**

**Lkhagvadulam, 김정화, \*윤일, \*\*심영기**

인제대 나노시스템공학과 \*인제대 PDT 연구소 \*\*인제대 나노공학부

We have synthesized a new type of water soluble ionic photosensitizer chlorin-p6 6-Ne-lysylamide -7-methyl ester. And it was transformed into a small gold nanoparticles stabilized by the photosensitizer without adding any particular reducing agents and surfactants. UV-Vis spectroscopy, Transmission Electron Microscopy (TEM), dynamic light scattering (DLS), TGA, XRD, <sup>1</sup>H-NMR, MS were used to confirm the formation of gold nanoparticles and photosensitizer. PDT Research Institute, School of Nano Engineering Systems, Inje University, Gimhae, KOREA, Correspondence to Y. K. Shim: (ykshim@inje.ac.kr)

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장소: 제주ICC

발표코드: III-MEDLP-224

발표분야: 의약화학

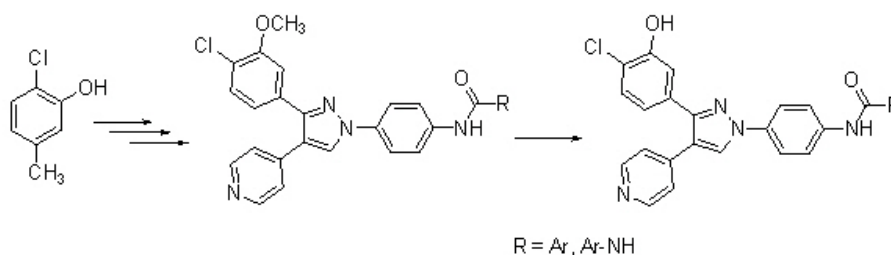
발표종류: 포스터, 발표일시: 금 10:30~12:30

## Synthesis and antiproliferative activity of new 1,3,4-triarylpyrazole derivatives against melanoma cell line

박이슬, \*Mohammed El-Gamal, \*\*유경호, \*\*조정혁, \*\*\*오창현

서강대 화학과 \*과학기술연합대학원대 Medicinal Chemistry \*\*KIST 생체과학연구본부 \*\*\*KIST  
바이오소재연구센터

Melanoma is the most aggressive form of skin cancer and is the fastest growing cancer in the United States. In this study, synthesis of a new series of diarylureas and diarylamides containing 1,3,4-triarylpyrazole scaffold is described. Their *in vitro* antiproliferative activity against A375 human melanoma cell line was tested and the effects of substituents on the triarylpyrazole scaffold were investigated.



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발표종류: 포스터, 발표일시: 금 10:30~12:30

## Synthesis of 123-I labeled benzopyran derivative

정순재, \*김인종, \*박정훈, \*\*김상욱, \*허민구, \*양승대, 유국현

동국대 화학과 \*한국원자력연구원 방사선기기연구부 \*\*동국대 나노소재화학화

The glutamate is the most abundant excitatory neurotransmitter in the vertebrate nervous system. The major function of glutamate receptor is a property of the brain thought to be vital for memory and learning. The overstimulation of glutamate receptor system (*N*-methyl-*D*-aspartate receptor) causes neurodegeneration due to a process called excitotoxicity such as Alzheimer's disease (AD). AD is the most common cause of dementia in the geriatric population. Benzopyran derivative has been having glutamate receptor antagonist in neurodegenerative diseases. In this study, we synthesized the I-123 labeled benzopyran derivative for neurodegeneration. The target compound was synthesized starting from 2-hydroxy-5-nitroacetophenone via six steps as a novel potential SPECT radiotracer for the diagnosis of neurodegenerative disorders. Further pharmacological investigation of I-123 labeled benzopyran derivative will be needed for clinical diagnosis of AD. But, I-123 labeled benzopyran derivative might have a potential to be utilized as a diagnosis agent for AD.

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장소: 제주ICC

발표코드: III-MEDLP-226

발표분야: 의약화학

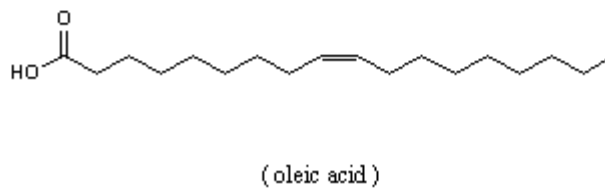
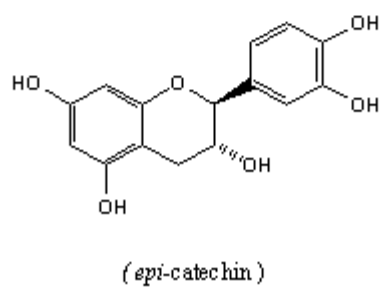
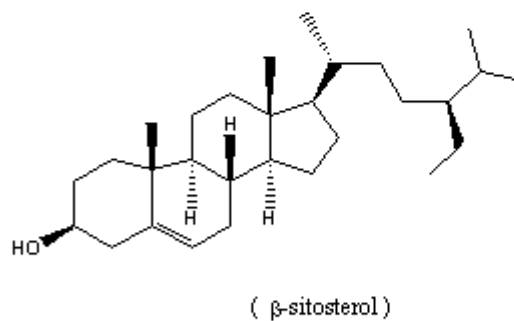
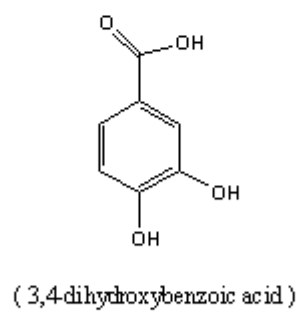
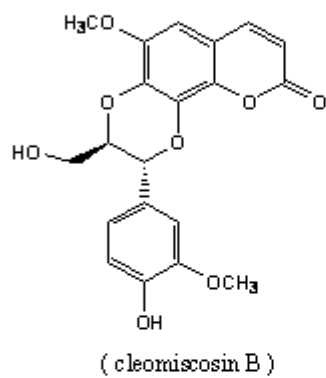
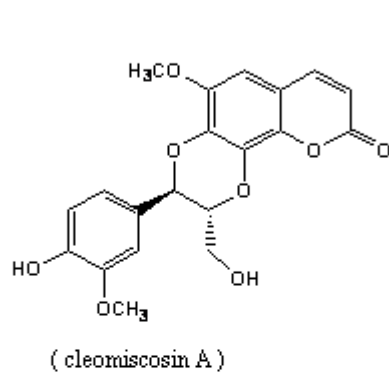
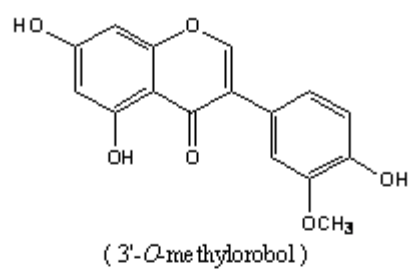
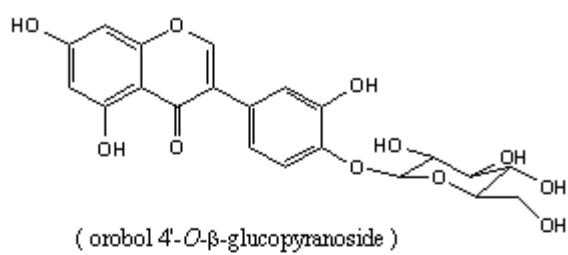
발표종류: 포스터, 발표일시: 금 10:30~12:30

## Antioxidative and Whitening Constituents from *Tilia taquetii* Branches

강유미, 양인정, 김수영, 이남호

제주대 화학과

Phytochemical investigation of the ethanol extract from *Tilia taquetii* stem by using repeated column chromatography, normal-phase silica gel and Sephadex LH-20, resulted in the isolation of eight compounds; orobol 4'-O- $\beta$ -glucopyranoside (1), 3'-O-methylorobol (2), cleomiscosin A (3), cleomiscosin B (4), 3,4-dihydroxybenzoic acid (5),  $\beta$ -sitosterol (6), *epi*-catechin (7) and oleic acid (8). Among these, the compound 1 is new, and the other compounds were isolated for the first time from *T. taquetii*. The isolated compounds were also subjected to the above biological tests. The compounds 7 (SC<sub>50</sub> 17.7  $\mu$ g/mL) and 2 (SC<sub>50</sub> 78.5  $\mu$ g/mL) showed good DPPH radical scavenging activities compared to ascorbic acid (SC<sub>50</sub> 7.7  $\mu$ g/mL) as a positive control. In addition, when DPPH and hydroxy radical scavenging activities were examined using ESR spectrometer, strong activities were observed in the compounds 5 and 7. For the tyrosinase inhibition test, the compounds 3 (IC<sub>50</sub> 12.9  $\mu$ g/mL) showed good activities compared to arbutin (IC<sub>50</sub> 104.6  $\mu$ g/mL) as a positive control. Based on the above experimental results, it is suggested that the extract from *Tilia taquetii* branches could be potentially applicable in cosmetic formulation as the functional, especially whitening ingredient.



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발표종류: 포스터, 발표일시: 금 10:30~12:30

## **The Discovery and synthesis of novel and potent allosteric mGluR1 antagonists for treating chronic pain.**

조경희, 정규성, \*배애님

연세대 화학과 \*KIST 생체과학연구본부

Metabotropic Glutamate Receptors have been studied that their physiological role is involved in the CNS and its possible pathophysiological processes. Thus, mGluRs are regarded as drug targets in order to modulate glutamate transmission in the treatment of various neurological and psychiatric diseases including pain, epilepsy, Parkinson's disease, cognitive disorders, drug abuse, anxiety and schizophrenia. The mGluR group I (subtype 1 and 5) is associated with pain transmission and drugs acting at this mGluR subtype might, therefore, be used in the treatment of chronic pain. We've expected potent and selective allosteric antagonists against mGluR1 having no side effect and good in vivo efficacy by diversity of structures. The design, synthesis and the biological activity against mGluR 1 will be presented.

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발표분야: 의약화학

발표종류: 포스터, 발표일시: 금 10:30~12:30

## Synthesis and Biological Evaluation of Serotonin Receptor Agonists as Antiobesity Agents

양하연, 태진성, \*배애님

연세대 화학과 \*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 19 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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발표분야: 의약화학

발표종류: 포스터, 발표일시: 금 10:30~12:30

## Development of Polo-like Kinase 1 Inhibitors to improve membrane penetration

윤선미, 유은경

한국기초과학지원연구원 자기공명연구부

Polo-like kinase 1 (Plk1) is overexpressed in human carcinomas has prognostic potential in cancer. It is an important regulator of cell cycle progression during mitosis. The polo-box domain (PBD) regulates the subcellular localization of plk1 during mitosis. The phosphopeptide, Pro-Leu-His-Ser-p-Thr (PLHSpT) has been reported as a potent and selective inhibitor of the PBD of human plk1 by apoptosis in cancer cells. However, it showed low membrane penetration of cell. Therefore, in these studies, we designed and synthesized Plk1 inhibitors of PLHSpT, such as folate-PLHSpT and RGD-S-S-PLHSpT, for improving internalization into cells. The folate-PLHSpT was prepared with folic acid (77 mg, 0.17 mmol) and PLHSpT linked resin (50 mg, 35  $\mu$ mol) with 4 equivalent of HBTU and HOBt, which are peptide coupling agents, in the presence of DIEA for 1 h at room temperature. SPDP was conjugated with lysine side chain of the protected RGDyK peptide under basic condition for 2 h in DMF. We synthesized the CPLHSpT using Fmoc-based solid-phase method on Rink amide resin (0.51 mmol/g). The RGD-S-S-PLHSpT was conjugated with activated RGD and CPLHSpT in DMF and then purified with HPLC. The folate- and RGD- fusion peptides were obtained with high chemical yield and purity. The compounds were identified by MALDI-TOF mass spectrometry. These fusion peptides were synthesized to be mediated by integrin or folate receptor for improving cell internalization. Further studies are warranted to investigate the biological evaluation of the novel fusion peptides in vitro cancer cell and in vivo tumor bearing animal models.



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발표종류: 포스터, 발표일시: 금 10:30~12:30

## Synthesis of indazole derivatives showing insecticidal activities

장성연, 임정연, 김성기

한국화학연구원 의약화학연구센터

Many anthranilamide insecticides are under development after the success of DuPont's chlorantraniliprole. Novel indazole derivatives containing anthranilamide moiety were synthesized and their insecticidal activities were evaluated. The amide coupling reaction of 2-amino-5-chloro-*N*,3-dimethylbenzamide and 2-(3-chloropyridin-2-yl)-2*H*-indazole-3-carboxylic acid in the presence of 3-picoline and methanesulfonyl chloride gave the most potent compound whose mortality against *Plutella xylostella* larvae was 95% at 100 ppm. Synthesis of indazole derivatives and their insecticidal activities will be presented.

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발표종류: 포스터, 발표일시: 금 10:30~12:30

## **Preparation of high molecular weight hyaluronic acid using fermentation & cross-linking methods**

신고은, 이동근, 이용규

충주대 화공생물공학과

Hyaluronic acid(HA) is a linear polysaccharide with repeating disaccharide units of glucuronic acid and N-acetylglucosamine and is found in the extracellular matrix of connective tissues. HA is an attractive building block for new biocompatible and biodegradable polymers with applications in drug delivery, tissue engineering, and viscosupplementation. Although it is soluble in water independently on its molecular weight, undergoes spontaneous depolymerization in solution, probably, due to some weak linkages related to N-acetylglucosamine in the chain. HA is natural biopolymer that have a great biocompatibility in body when it contacts with blood, body fluid and tissues. It can have various molecular weight that is due to special chemical property as occasion demands. Also, it is possible to reunion in body as enzyme and easy to reunion as regulation and cross-linking of functional group, hydrogel. In this work, we carried out optimization of medium components to produce high-molecular-weight HA in streptococcus eq. that lacked hemolytic activity and hyaluronidase industrially. Chemical modification allows the physicochemical properties and in vivo residence time of HA to be tailored to specific applications while retaining its natural biocompatibility, biodegradability, and lack of immunogenicity. The chemical bonding of the conjugates was characterized by <sup>1</sup>H-NMR, FT-IR.

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발표종류: 포스터, 발표일시: 금 10:30~12:30

## Synthesis and antitubercular activity of amino acid analogs

김경희, \*김수현, \*\*김필호, \*\*\*Helena Boshoff, \*\*\*Clifton E. Barry, \*\*\*\*오태권, \*\*\*\*\*이일영

한국화학연구원 난치성질환치로제연구센터 \*한국화학연구원 \*\*한국화학연구원 난치성질환치로제연구센터 \*\*\*Naional institutes of Health \*\*\*\*연세대 의과대학 \*\*\*\*\*한국화학연구원 감염증치료물질연구팀

In 2009, tuberculosis (TB) kills 1.7 million people including 380,000 people with HIV. One-third of the world's population is infected with Mycobacterium tuberculosis (Mtb), which causes TB. In the field of TB drug discovery, one of the most challenging questions to address is how to shorten the lengthy chemotherapy period: 6-9 months for drug-susceptible patients and 18-24 months for drug-resistant patients. Amino acid analogs have been utilized as anti-cancer and antibacterial agents. Recently we have discovered amino acid analogs active against Mtb. Design and synthesis of amino acid analogs will be presented. Structure-activity relationship of the prepared amino acid analogs against replicating and non-replicating Mtb will be also discussed.

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발표분야: 의약화학

발표종류: 포스터, 발표일시: 금 10:30~12:30

## PET Evaluation of Brain 5-HT<sub>1A</sub> Receptors in Rat in Vivo with Representative [<sup>18</sup>F]WAY Derivatives

최재용, \*김철훈, \*\*이치훈, \*\*한상진, \*\*김병수, \*\*최태현, 전태주, 유영훈

연세대 의과대학 강남세브란스병원 핵의학과 \*연세대 의과대학 약리학교실 \*\*한국원자력의학원 방사성의약품연구팀

The serotonin 1A (5-HT<sub>1A</sub>) receptors in the central nervous system are strongly associated in various neuropsychiatric disorders such as depression, anxiety and schizophrenia. Positron emission tomography (PET) as a non-invasive imaging technique with a high-sensitivity and quantitative property, provides the means to visualize receptor densities in living system. Thus, a number of PET radioligands are developed for measuring 5-HT<sub>1A</sub> receptor densities in the brain based on the WAY-100635. Among these derivatives, [<sup>18</sup>F]FCWAY, [<sup>18</sup>F]MPPF and [<sup>18</sup>F]MEFWAY are currently used in preclinical study. However, there have been few reports on the comparative study of these compounds. Here, we performed PET evaluation of brain 5-HT<sub>1A</sub> receptors in rat in vivo with these three compounds. For in vivo experiments, radioactivity (13.1 – 19.6 MBq) was injected to male Sprague-Dawley rat and fluconazole, antifungal drug was tested the a inhibitor of CYP2E1 to prevent defluorination. Regions of interest were hippocampus, frontal cortex (receptor-rich regions) and cerebellum (receptor-poor area). In conclusion, inhibitor treated [<sup>18</sup>F]FCWAY was the highest brain uptake and binding potential. From these result, we suggest that inhibitor treated [<sup>18</sup>F]FCWAY is the optimal PET radioligand in preclinical study.

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발표분야: 의약화학

발표종류: 포스터, 발표일시: 금 10:30~12:30

## Synthesis and Biological Evaluation of Novel T-type Calcium Channel Blockers for Treating Neuropathic Pain

임건승, 백두중, \*배애님

상명대 화학과 \*KIST 생체과학연구본부

T-type calcium channels are low voltage-activated(LVA) calcium channels and located in muscle, glial cell, neurons and SA node. It has been reported that T-type calcium channel blocker could be used for the treatment of epilepsy, obesity and neuropathic pain. Mibefradil(PosicorR), the first marketed selective T-type calcium channel blocker, was withdrawn due to toxicity because of the drug-drug interaction. Therefore, there have been a lot of efforts for developing T-type calcium channel blockers with new scaffolds and no side effect. As part of discovering novel T-type calcium channel blockers for the treatment of neuropathic pain, we designed oxazole and pyrrolidine derivatives and synthesized total 15 compounds. The synthesized compounds were biologically evaluated against T-type calcium channel. Here, we show the design, synthesis and biological evaluation of oxazole and pyrrolidine derivatives as T-type calcium channel blockers.

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발표종류: 포스터, 발표일시: 금 10:30~12:30

## Design and synthesis of 4-aminosalicylic acid (PAS) analogs as inhibitors of *Mycobacterium tuberculosis*

남보라, \*윤민한, \*\*강민서, \*김필호, \*\*\*Helena Boshoff, \*\*\*Clifton E. Barry, \*\*\*\*이일영

한국화학연구원 난치성치료제연구센터 \*한국화학연구원 난치성질환치료제연구센터 \*\*고려대  
화학과 \*\*\*National Institutes of Health \*\*\*\*한국화학연구원 감염증치료물질연구팀

4-aminosalicylic acid (PAS) has been used in the treatment of tuberculosis since 1946. For the demonstration of biological activity of PAS and obtaining substances with increased potency against the tubercle bacilli, a number of PAS derivatives have been synthesized but generally most of structural changes implicate a loss of activities. However, several substituted phenyl esters appear to be significantly more active than PAS. Thus, we initiated a program to prepare various phenyl esters to improve biological activity as prodrugs of PAS. The synthesis and activity as well as the structure-activity relationships of these compounds will be discussed.

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발표종류: 포스터, 발표일시: 금 10:30~12:30

## Synthesis and evaluation of 2-arylsulfanyl and sulfonyl substituted 5,6-dihydro-pyrrolo[3,4-b]pyridin-7-one derivatives as MCH receptor 1 antagonist

임채조, 이은경, 이규양, 김지영, \*이가은

한국화학연구원 대사증후군치료제연구센터 \*과학기술연합대학원대 의약및약품화학

Since the melanin-concentrating hormone receptor (MCH-R1) was known as an important role in the regulation of food intake and energy balance, MCH antagonists have been considered as a potential therapeutics for the treatment of obesity. In continuation of our efforts to search for new scaffolds of MCH-R1 antagonists, we have identified a series of 5,6-dihydro-pyrrolo[3,4-b]pyridin-7-one derivatives and examined the effect of various arylsulfanyl and sulfonyl and group at 2-position of 5,6-dihydro-pyrrolo[3,4-b]pyridin-7-one to the MCH-R1 binding activity. The details of synthesis and binding affinity will be presented.

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## **A Novel Class of DAXX nuclear export inhibitors; Synthesis and biological evaluations of benzothiophenecarboxylic acid amide and naphtho[1,2-b]furan carboxylic acid amide derivatives**

이서현, 서지희, 이규양, \*김수희

한국화학연구원 대사증후군치료제연구센터 \*과학기술연합대학원대 의약및약품화학

DAXX is a Fas-binding proapoptotic protein that is a component of the death-inducing signaling complex in Fas-mediated apoptosis. During ischemic stress, Daxx translocates from the nucleus to the cytoplasm. The cytoplasmic presence of Daxx is essential for cell death upon ischemic insult. As part of our efforts to find new scaffolds of DAXX nuclear export inhibitors as effective anti-ischemic agents, we have designed and synthesized a series of benzothiophenecarboxylic acid amide and naphtho[1,2-b]furancarboxylic acid amide derivatives. Synthesized compounds were biologically evaluated using in vitro H9c2 cell. Pharmacological activities correlated with their structures will be presented.



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발표종류: 포스터, 발표일시: 금 10:30~12:30

## Evaluation of Size Dependant In vivo Tumor Targetability using PEGylated Mesoporous Silica Nanoparticle.

박주영, 김혜란, 김동욱

전북대 의과대학 핵의학과

Purpose : In this study, we developed various size of mesoporous silica nanoparticle (MSN) for tumor optical fluorescence imaging. The accumulation in the tumor tissue of MSN was occurred through enhanced permeability and retention (EPR) mechanism. Method : MSN were synthesized by a self-assembly method and this surface was covered with amine terminal. Particle size was regulated with NaOH. This MSN was conjugated with hydroxysuccinimidyl-PEG (Mw: 685.71) (MSN-PEG) and then hydroxysuccinimidyl-Cy5.5 (MSN-PEG-Cy5.5). TEM, FT-IR and pore size distribution of MSN-PEG were determined. For in vivo studies, various size of MSN-PEG-Cy5.5s were injected via tail vein into U87MG xenografted mice. Images were acquired until 24 h after post-injection. Results : Size distribution of MSN-PEG-Cy5.5s was from 30 to 170 nm (30, 60, 100, and 170). TEM images showed the highly uniform characteristics in terms of both particle size and shape. IVIS in vivo optical images showed that MSN-PEG-Cy5.5s with 100 or 170 nm were more highly accumulated in the liver and tumor over time compared with MSN-PEG-Cy5.5s with 30 or 60 nm. Ex vivo images of MSN-PEG-Cy5.5s with 100 or 170 nm were also showed high signal intensity in the tumor tissue than MSN-PEG-Cy5.5s with 30 or 60 nm. Conclusion : These results suggest that in vivo tumor accumulation of MSN-PEG-Cy5.5s through enhanced permeability and retention (EPR) mechanism was increased with particle size dependently. The design of particle size will be an important factor and so should include a careful consideration of the effect size upon MSN used for therapeutic carrier to delivery an anticancer drug.

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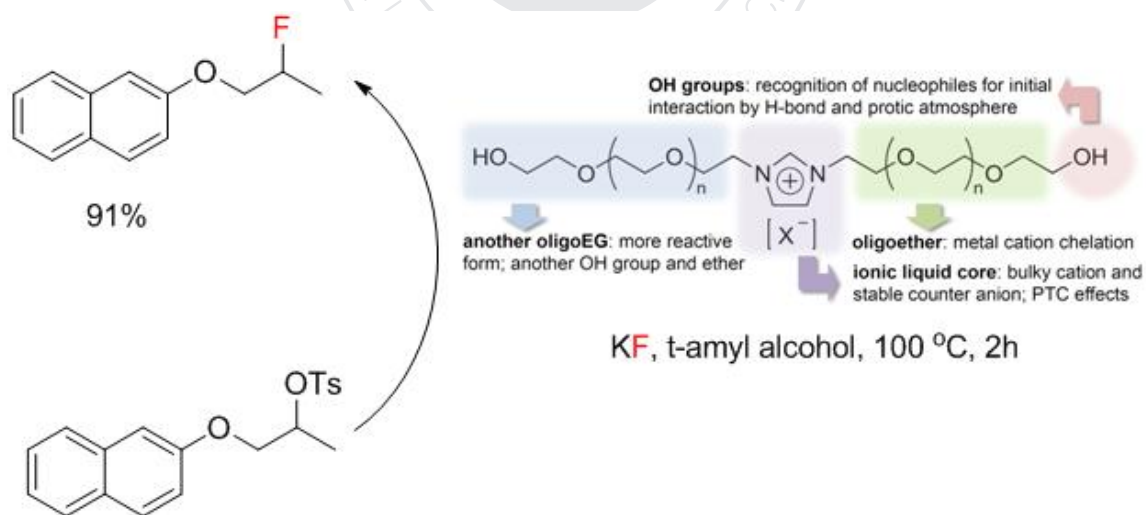
발표종류: 포스터, 발표일시: 금 10:30~12:30

## Tailor-Made Hexaethylene Glycolic Ionic Liquids as Organic Catalysts for Specific Chemical Reactions

JADHAV VINOD HANMANT, 이상봉, 김동욱

전북대 핵의학과

We have designed and prepared hexaethylene glycols substituted imidazolium based ionic liquids (hexaEGILs) well-tailored to the specific organic reaction using alkali-metal fluoride (MF) as multifunctional organic catalysts. These hexaEGILs catalyst could enhance the reactivity of MF, even KF, significantly. Furthermore, the hexaEGIL systems showed tremendous efficiency in the nucleophilic fluorination of base-sensitive substrates.



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발표종류: 포스터, 발표일시: 금 10:30~12:30

## Synthesis of $^{18}\text{F}$ -labeled Compound from Gold/CopperSurface-bound Sulfonate Precursor

장승호, kalme sachin, 김동욱

전북대 의과대학 핵의학과

Thiol and disulfide compounds were adsorbed on gold/copper surface, sulfonate compounds were very useful precursors for  $^{18}\text{F}$ -labeled radiotracers in PET. Radiolabeling method by using solid supported precursor is easy to purify after radiolabeling. A new approach to the  $^{18}\text{F}$ -labeling method is described, which employs supported disulfide-sulfonate precursors, where the support gold/copper surface.

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## Functionalized Graphene Oxide-Polysaccharide Conjugate for Improved Blood Compatibility

김유진, 백기선, \*인인식, 이용규

충주대 화공생물공학과 \*충주대 나노고분자공학과

Graphene is a single atomic layer of  $sp^2$  carbon atoms. Graphene has received increasing interests due to its fascinating electrical, thermal, and mechanical properties in various applications. However, biological application of graphene is unexplored. So, we explore the biological applications of graphene oxide. Blood compatibility is one of the important and critical issues when nanomaterials such as nanoparticles. So, Synthesis of polysaccharide and GO for improved blood compatibility were designed a esterification. The chemical bonding of the synthesis was characterized by Raman spectrum, dynamic light scattering(DLS), SEM, FT-IR and UV-vis spectroscopy. According to this study, we known graphene oxide is new material of biological and medical application.

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발표분야: 의약화학

발표종류: 포스터, 발표일시: 금 10:30~12:30

## Analysis for Different Activities of 11 $\beta$ -HSD1 Inhibitors in the Human and Mouse Species

이주연, 강남숙

한국화학연구원 신약플랫폼기술팀

11 $\beta$ -Hydroxysteroid dehydrogenase type 1 (11 $\beta$ -HSD1) catalyzing the intracellular activation of cortisone to cortisol is currently considered a promising target to treat patients with metabolic syndrome, hence there is considerable interest in the development of selective inhibitors. Many researchers have some difficulties in identifying compounds that are equivalently active towards both human and rodent 11 $\beta$ -HSD1 enzymes. Our aim was to build the models that can show differences of structural features in human and rodent 11 $\beta$ -HSD1 enzymes using in-house compounds as potential 11 $\beta$ -HSD1 inhibitors. It is possible to get new insights into the structural relationship a series of compounds with human and rodent 11 $\beta$ -HSD1 enzymes.

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발표코드: III-MEDLP-243

발표분야: 의약화학

발표종류: 포스터, 발표일시: 금 10:30~12:30

## Novel resveratrol derivatives with axial chirality from seed of Iris Pseudacorus

최춘환, \*차미란, \*\*김영섭, \*\*\*연규환

충남대 약학 \*충남대 약학대학 \*\*한국화학연구원 신약연구단 \*\*\*한국화학연구원 화학물질연구  
단

The ethanol extract from the seed of Iris pseudacorus (Iridaceae) demonstrated a potent inhibition on the proliferation of four cultured human cells such as A549, SK-OV-3, SK-MEL-2 and XF498 in vitro. Three new resveratrol derivatives, Irisferin A-C (1 - 3) together with 5 known resveratrol oligomers were isolated from the extract. as active principles responsible for the cytotoxic effect on tumor cells, in vitro. The chemical structures of 1 - 3 were elucidated by extensive spectroscopic analyses especially 2D (COSY, HMQC, HMBC and ROESY) NMR data and HR-FABMS data. The absolute configuration of compounds (1 - 3) was determined by the comparison between experimental CD spectra of 1 - 3 and theoretical ECD(quantum chemically simulated electronic circular dichroism) spectra of corresponding compounds, which was calculated by time-dependent density functional theory (TDDFT : Gaussian 03). All resveratrol derivatives (1-8) exhibited significant inhibition on the proliferation of cultured human cells such as A549, SK-OV-3, SK-MEL-2 and XF498, in a dose dependent manner, respectively.

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발표종류: 포스터, 발표일시: 금 10:30~12:30

## A Novel 3-Phenylethynyl-2-yl-oxy Quinoxaline Core Skeleton and Pharmacophore Model as a Hypoxia-inducible Factor Inhibitor

배미선, 공영대, \*강남숙

동국대 화학과 \*한국화학연구원 신약플랫폼기술팀 분자설계

The importance of HIF-1 $\alpha$  in the mediation of normal and pathological processes has motivated considerable efforts to identify HIF-1 $\alpha$  inhibitors. Although a wealth of inhibitory compounds is available, synthesizing HIF-1 $\alpha$  inhibitors with a novel small-molecule core skeleton fitting individual HIF-1 $\alpha$  has proven to be a challenge. Here, we report initial evidence showing that compounds with a 3-Phenylethynyl-2-yl-oxy quinoxaline core skeleton are selective HIF-1 $\alpha$  inhibitors, and therefore have potential to be anticancer agents. The aim of this study was to investigate the biochemical properties of HIF-1 $\alpha$  and identify new core skeleton inhibitors of HIF-1 $\alpha$ . To identify small-molecule inhibitors of HIF-1 $\alpha$ , we screened 163 substituted quinoxaline derivatives using the HRE/SW480 stable cell line containing HRE-luc[pHTS-9XHRE-Luc]. The 163 screened quinoxaline compounds represent 4,000 structurally diverse and druggable derivatives.

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## **A -Novel 3-(8-Chloro-6-(trifluoromethyl)imidazo[1,2-a]pyridine-2-yl)phenyl Acetate Skeleton and Pharmacophore Model as Glucagon-like Peptide 1 Receptor Agonists**

김나연, 김지혜, 공영대, \*강남숙

동국대 화학과 \*한국화학연구원 신약플랫폼기술팀 분자설계

The recent discovery of the nonpeptidic glucagon-like peptide 1 receptor (GLP-1R) agonists has attracted strong research attention as it has the potential to offer a magic bullet treatment for diabetes. Exploitation of the incretin GLP-1P has afforded effective pharmacological agents for the treatment of diabetes. The importance of GLP-1R in the mediation of normal and pathological processes has motivated considerable efforts to identify GLP-1R agonists. Although a wealth of activator compounds are available, synthesizing small-molecule GLP-1R agonists with a novel core skeleton fitting individual GLP-1R agonists with a novel core skeleton fitting individual GLP-1R have proven to be a challenge. Therefore, we undertook an investigation aimed at developing novel and simple drug-like heterocyclic derivatives as GLP-1R agonists. Herein, We report initial evidence showing that compounds with a 3-(8-chloro-6-(trifluoromethyl)imidazo[1,2-a]pyridine-2-yl)phenyl acetate moiety are selective GLP-1R agonists, and have potential as anti-diabetic treatment agents. To aim of this study was to investigate the biochemical properties of these GLP-1R agonists and identify their new core skeleton. We screened 1000 compounds and identified 3-(8-Chloro-6-(trifluoromethyl)imidazo[1,2-a]pyridine-2-yl)phenyl acetate skeleton, as the GLP-1R agonist



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발표종류: 포스터, 발표일시: 금 10:30~12:30

## Solid-phase Synthesis of 5-Phenyl-(4-amino substituted)Oxadiazole Derivatives via Thiourea Linker on BAL Resin

양승주, 이석형, 김나연, 공영대

동국대 화학과

Heterocyclic skeletons serve as the core components of a large number of substances that possess a wide range of interesting biological activities. And 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 oxadiazole 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 oxadiazole through resin-bound thiourea linker on BAL resin. The 5-Phenyl-(4-amino substituted)oxadiazole derivatives have attracted much attention for their interesting biological activities such as COX-2, 5-LO, and various receptor antagonists. Through making the piperazine, we can obtain linear compound. And this linear heterocyclic compound can act as kinase inhibitor. The final compounds were obtained in good yields and high purities upon cleavage from the resins.

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## **Solid-Phase synthesis of 2-Amido/Amine Substituted Benzo[d]oxazole Derivatives via Thiourea Linker on BAL Resin.**

정세린, 김슬기, 곽현정, 공영대

동국대 화학과

Solid-phase synthesis of combinatorial libraries has emerged as a powerful tool for efficient drug discovery process. As a part of an ongoing drug discovery program, we have been exploring the potential of resin-bound benzo[d]oxazole derivatives as a versatile intermediate for generation of drug-like heterocyclic compound libraries. Especially, we were interested in construction the variously substituted 2-amido/amine substituted benzo[d]oxazole library because of their broad biological activities. Further diversification can be introduced to a benzo[d]oxazole-5-amine resin, derived from the nitro group containing resin. Herein we would like to present novel solid-phase synthetic method for combinatorial generation of benzo[d]oxazole based library through resin-bound BAL linker. The final compounds were obtained in good yields and high purities upon cleavage from the resins.

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## **Solid-phase synthesis of a novel drug-like 2-thioxoimidazolidine-4-one derivatives via benzyl thiocyanate linker**

이지형, 이재민, 배미선, 공영대

동국대 화학과

Solid-phase synthesis of heterocyclic combinatorial libraries has emerged as a powerful tool for efficient 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 there 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-thioxoimidazolidine derivatives have attracted much attention for their interesting biological activities such as Hif-1 $\alpha$  and Wnt signal path way, and various receptor antagonist. Through making the various substituted aromatic building blocks, we can obtained linear compound. And this linear heterocyclic compound can act as Hif-1 $\alpha$  or Wnt signal path way. The final compound were obtained in good yield and high purities from solution-phase synthetic process.

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## Discovery of anti-HIV drugs at Institut Pasteur Korea

김준원, \*이두현, \*\*권정진, \*\*\*공선주, 조수연, \*\*노재성

한국파스퇴르연구소 의약화학팀 \*한국파스퇴르연구소 의약화학 \*\*한국파스퇴르연구소 \*\*\*한국  
파스퇴르연구소 의약화학실

Although an unprecedented success has been achieved in discovering anti-HIV drugs, the use of these drugs has been relatively limited by their toxicity, drug resistance development, and more worryingly, the fact that some newly HIV-infected patients carry viruses that are already resistant to the currently approved AIDS treatments. These issues along with drug-related side effects as well as poor tolerability of current drugs make it apparent that new anti-HIV drugs with acceptable toxicity and resistance profiles, and, more importantly, new anti-HIV agents with novel mechanism of action are clearly needed. For the HIV drug discovery program, we have been working on NNRTI and novel targets. We have found the scaffold-A is targeting an allosteric binding site of reverse transcriptase. The scaffold-A derivatives show clear SAR in cell-based assay and comparable activities against RT mutants. Together the promising mutant profile, good rat in vivo PK, and hERG & P-gp inhibition results prompted us to pursue dog in vivo PK and acute toxicity tests. For the HIV novel target program, we have found several HITs that are not active against known target assays. One of them, the scaffold-B is clearly working on the early entry step, which we confirmed by target identification assay. Along with focused SAR, more biological evaluations are under investigation.

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## Synthesis and evaluation of 2,5-Disubstituted Aryl 2H-Pyridazinone derivatives as Androgen Receptor(AR) Antagonists

김낙정, \*김성환, \*\*강남숙, \*\*\*백승화, 이규양, 서지희, 임채조

한국화학연구원 대사증후군치료제연구센터 \*한국화학연구원 화학유전체 연구실 \*\*한국화학연구원 신약플랫폼기술팀 분자설계 \*\*\*한국화학연구원 약리활성연구실

The Androgen receptor(AR) is an important member of the superfamily of nuclear hormone receptors that functions as ligand-dependent regulator of transcription. The AR antagonists are useful in treatment of prostate cancer, benign prostate hyperplasia, alopecia, breast cancer and acne. As novel AR antagonists, we have designed and synthesized a series of 2,5-Disubstituted aryl 2H-pyridazinone derivatives. Among them, some of these compounds exhibited a potent activity in LNCaP/PC-3 cell based assay. The details of synthesis and biological efficacy will be presented.

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## Desing and synthesis of Selective Inhibitors for Cytochrome P450 1B1

장원영, 임채민, 김창훈, 김상희

서울대 약학과

The cytochrome P450 subfamily 1 (CYP1) has long been of interest to researchers because of its relevance to carcinogenesis. The human CYP1 family contains three members, CYP1A1, CYP1A2, and CYP1B1. Among these, CYP1B1 has received considerable attention as a new drug target. So we designed and synthesized 3,5-dimethoxyphenyl moiety through solution phase synthetic pathway, and their inhibitory activities were evaluated on human cytochrome P450s (CYP) 1A1, 1A2, and 1B1 to find a potent and selective CYP1B1 inhibitor. Among the compounds tested, the most selective and potent CYP1B1 inhibitor was 2,3',4,5'-tetramethoxystilbene. Moreover we found that 2-Methoxy group in stilbene plays crucial role for discriminating between CYP1As and CYPB1.

On the basis of our previous studies, We prepared 2,4-dimethoxy group containing stilbenes for effects on the activity of CYP1s with the ultimate goal of identifying a potent and selective CYP1B1 inhibitor. Five compounds exhibited similar or greater potency in inhibiting CYP1B1 compared to the previous 3,5-dimethoxyphenyl moiety. Molecular modeling was performed to determine the key molecular interactions with the CYP1B1 and CYP1A2 structures. On the basis of these structural and biological studies, the design of more potent and more selective drug-like derivatives can be envisaged

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발표종류: 포스터, 발표일시: 금 10:30~12:30

## Synthesis of stereoisomers of D-ribo-Phytosphingosine via a Cyclic Sulfate and Bis-Sulfonate Intermediate

이윤미, 조지희, 이석우, 전홍준, 김상희

서울대 약학대학

The growing interest in the biological functions of sphingolipids has generated a need to develop efficient methods for the preparation of the stereoisomers of sphingoid base, phytosphingosine. In the course of our ongoing research, we have explored efficient route for the transformation of cheap, commercially available D-ribo-phytosphingosine into other stereoisomers.

Herein, we wish to report our successful synthesis of D-xylo- and D-lyxo- phytosphingosines from D-ribo-phytosphingosine based on the configurational inversion of the stereocenter via a regioselective nucleophilic substitution of a cyclic sulfate and bis-sulfonate. We found that the thermolysis of the cyclic sulfate led to an inversion of configuration of the proximal hydroxyl group, whereas the bis-sulfonate led to an inversion of configuration of the distal hydroxyl group. This study allowed us to compare a cyclic sulfate and a bis-sulfonate in an intramolecular substitution reaction.

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발표분야: 의약화학

발표종류: 포스터, 발표일시: 금 10:30~12:30

## Synthesis and Evaluation of Pachastrissamine Analogs

전홍준, 이석우, 이윤미, 김상희

서울대 약학대학

Pachastrissamine which was isolated in 2002, is a naturally occurring anhydrophytosphingosine which has attracted much attention from synthetic chemists in recent years. Since it exhibits potent cytotoxic activity against various human carcinoma cell lines, we have been prompted to achieve the stereoselective synthesis of analogues of pachastrissamine from phytosphingosine. These analogues differ from original structure of pachastrissamine in that the atom of oxygen of pachastrissamine is substituted to sulfur and nitrogen, respectively. So, we synthesized the designed analogues from phytosphingosine via 7-membered cyclic sulfate intermediate.



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## Synthesis and evaluation of deoxygenated $\alpha$ -GalCer analog

김재현, 이지민, 권용석, 김상희

서울대 약학과

$\alpha$ -GalCer, a structurally modified analogue of the marine natural product agelasphins, is the first defined and potent agonist for natural killer T (NKT) cells. Along with the observed hydrogen-bonding interactions in the crystal structure, previous SAR studies on the phytosphingosine moiety of  $\alpha$ -GalCer led to consider that the 3-hydroxyl group of phytosphingosine is a crucial group to activate NKT cells and the 4-hydroxyl group is not crucial to activity. However, the analog lacking only the 3-hydroxyl group on the phytosphingosine (3-deoxy  $\alpha$ -GalCer) has not been synthesized and evaluated. Here in, we present the synthesis and preliminary evaluation of 3-deoxy  $\alpha$ -GalCer.

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발표분야: 의약화학

발표종류: 포스터, 발표일시: 금 10:30~12:30

## Silver-Mediated *exo*-Selective Tandem Desilylative Bromination/Oxycyclization of Silyl-Protected Alkynol

이현지, 임채민, 황순호, 김상희

서울대 약학과

The exocyclic  $\beta$ -bromo enol ether is a synthetically useful functional moiety in the preparation of functionalized oxygen heterocycles because it contains both a vinyl halide moiety and an enol ether functionality on the periphery of the oxygen heterocycle. This synthetically valuable moiety has previously been accessible primarily through a stepwise conversion of the appropriate substrate. We envisioned that this functional moiety could be obtained directly from the silylacetylenic alcohols via tandem silver(I)-mediated desilylative bromination and heterocyclization. We found that the AgF/NBS system was effective for this purpose. To demonstrate the synthetic potential of the developed method, a brief total synthesis of pachastrissamine was successfully attempted.

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발표분야: 의약화학

발표종류: 포스터, 발표일시: 금 10:30~12:30

## Preparation and Characterization of 3-[<sup>131</sup>I]iodo-L-tyrosine grafted CoFe<sub>2</sub>O<sub>4</sub>@SiO<sub>2</sub> nanoparticles for Single Photon Emission Computed Tomography (SPECT) and Magnetic Resonance Imaging (MRI)

조보배, 유국현

동국대 화학과

Recently, the design of surface modified nanoparticles have been interested greatly due to the major applications in nanobiotechnology. Among the various nanoparticles, iron oxide was used to have applications in tagging for biosensing, probe of drug delivery and contrast reagent for magnetic resonance imaging (MRI). Especially, combined imaging system of single photon emission computed tomography (SPECT) with MRI provides more clear images for diagnostic use. In this study, we have successfully developed 3-iodo-tyrosine grafted CoFe<sub>2</sub>O<sub>4</sub>@SiO<sub>2</sub> nanoparticles as a novel imaging agent for simultaneous detection of tumor in SPECT and MRI. Monodispersed CoFe<sub>2</sub>O<sub>4</sub> nanoparticles were synthesized through thermal decomposition of Fe(acac)<sub>3</sub> and Co(acac)<sub>2</sub> (acac=acetylacetonate). CoFe<sub>2</sub>O<sub>4</sub>@SiO<sub>2</sub> core shell structure was prepared by reverse microemulsion. After aminopropyl triethoxysilane modification on the surface of obtained nanocomposites, L-tyrosine molecules were introduced by simple amide coupling method. Finally, surface attached L-tyrosine molecules are labelled to 3-[<sup>131</sup>I]iodo-L-tyrosine by aromatic iodination with Na<sup>131</sup>I. <sup>131</sup>I - it is widely used for SPECT - was easy to gain that is by-product from nuclear reactor 'hanaro' compare to other products from the cyclotron like as <sup>123</sup>I or <sup>124</sup>I. The physicochemical characterizations (XRD, TEM, FT-IR, TG, Elemental analysis,  $\gamma$ -ray detection) on obtained nanocomposites have been carried out. This bi-functional imaging agent may allow to earlier detection of tumor with a high degree of accuracy

일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: III-MEDLP-257

발표분야: 의약화학

발표종류: 포스터, 발표일시: 금 10:30~12:30

## Synthesis and Biological Evaluation of 5-Substituted Pyrazole Derivatives as Calcium Channel Inhibitors

김정현, 남길수, 최경일

KIST 생체과학연구본부

Inhibition of calcium channels is heralded as a potential treatment to peripheral and CNS disorders, including hypertension, heart failure, sleep disorder, epilepsy, drug addiction and neuropathic pain. As an effort to develop potent calcium channel inhibitors, we have been studying various pyrazole derivatives. Here the synthesis and biological evaluation ( $\alpha 1G$ ,  $\alpha 1H$  calcium channels and hERG channel blocking activity) of a series of 5-substituted pyrazole derivatives will be discussed.

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발표분야: 의약화학

발표종류: 포스터, 발표일시: 금 10:30~12:30

## Preparation of radio-iodine labeled stilbene derivative and its distribution in mice

김병수, 이치훈, \*하형호, 한상진, 안광일, \*이승찬, \*장영태, 최태현

한국원자력의학원 방사성의약품연구팀 \*National University of Singapore

Some stilbene derivatives have been reported for detection of A $\beta$  ( $\beta$ -amyloid peptide) fibrils, which is one of major component of peptide/protein deposits in Alzheimer's disease (AD), in vitro. Here, we prepared radio-iodine labeled stilbene derivative (3'-ISB, 4-(N-methyl-N-2-hydroxyethyl)-3'-[ $^{125}$ I]iodostilbene) from its tributyltinyl- precursor. For the purpose of assessment of brain distribution we further investigated in vivo distribution of radio-iodinated stilbene derivatives in mice using whole body autoradiography technique. Radio-iodinated stilbene derivative (3'-[ $^{125}$ I]ISB) was prepared by nucleophilic substitution between oxidized radio-iodine and tributyltinyl group. The reaction product was purified by preparative HPLC. The stability of 3'-[ $^{125}$ I]ISB in saline was assessed under various storage condition (RT, 4°C and -20°C) for a week. Whole body autoradiograms were acquired after single i.v. bolus 3'-[ $^{125}$ I]ISB injection of 4 MBq/kg dose in male ICR mice. The distribution of radio-activity was analyzed by BAS5000 imaging analyzer system. The radio-labeling yield of 3'-[ $^{125}$ I]ISB was 51.1%. After purification by preparative HPLC, the final recovery and radio-chemical purity were approximately 25% and 99.4%, respectively. The radio-chemical purity followed a week storage at RT, 4°C and -20°C was 72.3%, 71.3% and 57.6%, respectively. compound was most unstable in saline where it stored at -20°C. But, the radio-labeled compound was stable at room temperature and 4°C for a day. In whole body autoradiograms followed single i.v. bolus injection of 3'-[ $^{125}$ I]ISB, the moderate level of radio-activity was found in brain. Purified radio-iodinated stilbene derivative (3'-[ $^{125}$ I]ISB) was successfully prepared. The radio-labeled compound was most unstable in saline where it stored at -20°C. But, the radio-labeled compound was stable at room temperature and 4°C for a day. Whole body autoradiograms showed that the stilbene derivative can pass the brain-blood barrier and can be a potential imaging probe for A $\beta$ .

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장소: 제주ICC

발표코드: III-MEDLP-259

발표분야: 의약화학

발표종류: 포스터, 발표일시: 금 10:30~12:30

## Physicochemical Profiling in Drug Discovery

우재춘, 채종학, 김선우, 안성훈, 배명애

한국화학연구원 신약플랫폼기술팀

물성분석기술은 신약개발 초기단계에서 화합물의 물리화학적 성질의 스크리닝을 통해 ADME/Tox 에 영향을 미치는 주요 성질들을 조기에 해석할 수 있도록 하는 기술이다. 한국화학연구원에서는 국내 신약개발연구 초기단계에서 물성 최적화 연구를 통하여 고품질의 선도물질 선별, 연구의 집중화를 통하여 신약개발의 성공률을 높이고 신약개발연구의 선진화를 위하여 기본 물성 평가시스템을 도입하였다. 이를 기반으로 범국가차원의 물성평가연구 인프라를 구축하고 물성평가 연구의 전문화와 표준화에 노력하여 국내 제약산업의 영세성극복을 위한 공동활용 및 지원을 목표로 본연구팀에서는 integrity, pKa, lipophilicity, solubility 및 permeability 등 기본 물성항목에 역점을 두어 기존 기술을 업그레이드하고 신기술 도입 및 개발 연구를 추진중이다.

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발표코드: III-MEDLP-260

발표분야: 의약화학

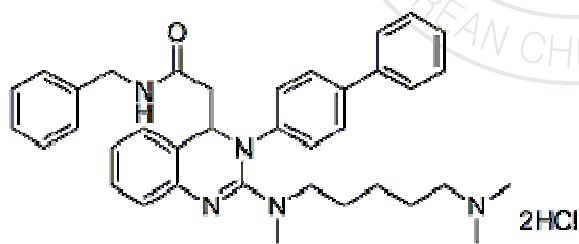
발표종류: 포스터, 발표일시: 금 10:30~12:30

## Pharmacokinetic Profile and Antitumor Activity of 3,4-Dihydroquinazoline Derivatives As Novel Anti-cancer Agents

강한별, 박진영, 최홍우, 주동준, 이재열

경희대 화학과

In the previous work, we have reported that 3,4-dihydroquinazoline derivatives are potent and selective T-type calcium channel blockers that exhibited strong anti-cancer activity in vitro. Among them, Compound 1•2HCl was further in vivo evaluated against A549 xenograft in BALB/c nude mice, which exhibited 49% tumor-weight inhibition through intravenous administration of 2 mg/kg of body weight and was more potent than doxorubicin. Moreover, compound 1•2HCl has an oral bioavailability of 98% with LD50 values of 963 mg/kg (po route) and 40.0 mg/kg (iv route) of body weight.



**3,4-Dihydroquinazoline (1)**

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장소: 제주ICC

발표코드: III-MEDLP-261

발표분야: 의약화학

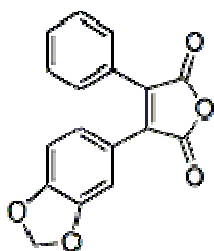
발표종류: 포스터, 발표일시: 금 10:30~12:30

## Synthesis and Biological Evaluation of 3-(Benzo[d]-1,3-dioxol-5-yl)-4-phenylfuran-2,5-dione as A New Anti-Inflammation Agent

김태우, 이기재, 성석봉, 주동준, 이재열

경희대 화학과

3,4-Diphenyl-substituted 1H-furan-2,5-dione and 1H-pyrrole-2,5-dione derivatives were synthesized using one of three synthetic methods and evaluated for the inhibitory activities on lipopolysaccharide (LPS)-induced PGE2 production in RAW 264.7 macrophage cells. Among them, 3-(benzo[d]-1,3-dioxol-5-yl)-4-phenylfuran-2,5-dione (5a) (BPD) was found to significantly inhibit LPS-induced PGE2 production in RAW 264.7 cells. This result is consistent with the following biological data: BPD not only reduced the LPS-induced expression of cyclooxygenase-2 (COX-2) at the protein and mRNA levels, but also inhibited COX-2 activity. Furthermore, BPD attenuated LPS-induced DNA binding activity and the transcription activity of activator protein-1(AP-1) and nuclear factor-kappa B (NF-κB).



**3-(benzo[d]-1,3-dioxol-5-yl)-4-phenylfuran-2,5-dione (BPD)**



일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: III-MEDLP-262

발표분야: 의약화학

발표종류: 포스터, 발표일시: 금 10:30~12:30

## **Synthesis and biological activities of (R) or (S) -1-(4-halophenyloxy)-3-(4-substituted piperazine-1-yl)propan-2-ol derivatives as T-type calcium channel blockers**

노은주

KIST 생체과학연구부

A series of compounds were designed as T-type calcium channel blocker from ligand based virtual screening. To obtain focused library based on the suggested structure, derivatives were synthesized then their inhibitory activities on T-type calcium channel were assayed using in vitro screening system. As a result of in vitro inhibition assays, several compounds showed as good inhibitory activities as mibefradil. Among the new 1-(2-hydroxy-3-phenoxypropyl) piperazine derivatives, 3d and 3f exhibited good selectivity for T-type  $\text{Ca}^{2+}$  channel against hERG channel. Therefore, in vivo efficacy was measured using neuropathic pain animal model.

일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: III-MEDLP-263

발표분야: 의약화학

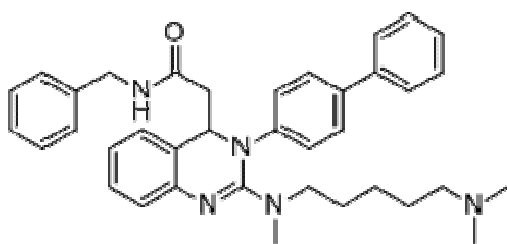
발표종류: 포스터, 발표일시: 금 10:30~12:30

## A New Synthetic Procedure to 3,4-DihydroquinazolineAs A Novel Anti-cancer Agent

박진영, 강한별, 최홍우, 주동준, 이재열

경희대 화학과

3,4-Dihydroquinazoline derivative (1•2HCl) as T-type channel blocker was found to exhibit the strong growth inhibitory effect against A549 xenograft in BALB/c nude mice. These in vivo results revealed that compound 1•2HCl could be a promising treatment in anti-cancer therapy. However, our previously reported procedure had a few of synthetic problems for compound 1, which required multi-step reactions, high expensive reagents and unstable intermediates. Therefore, a more efficient synthetic procedure should be desired to furnish the quantities of compound 1 required for further in vivo biological evaluation study. Herein, an efficient and economical synthetic procedure for compound 1 will be described.



**3,4-Dihydroquinazoline (1)**

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발표코드: III-MEDLP-264

발표분야: 의약화학

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## Discovery of Anti-Tuberculosis (TB) Drugs at Institut Pasteur Korea (IP-Korea)

김재승, 강선희, 서민정, 이세연, 김영미, \*고윤애, \*\*노재성

한국파스퇴르연구소 의약화학그룹 \*한국파스퇴르연구소 의약화학 \*\*한국파스퇴르연구소

Tuberculosis (TB), caused by *Mycobacterium tuberculosis* (Mtb) is a leading cause of death worldwide. Recent statistics from WHO estimate that there are approximately 9.2 million new TB cases every year with a global mortality rate of 23%. Poor patient compliance due to the cost of drugs, adverse effects, long time required for full treatment (6–12 months). Non-compliance has contributed to the appearance of multi-drug resistant (MDR) and extensively drug resistant (XDR) TB strains. Therefore, there is an urgent need for the development of new anti-TB drugs with novel target(s), which are active against drug-resistant as well as drug-sensitive TB strains. TB program at IP-Korea established cell-based imaging technology and integration of process functions (Screening platform, Biology, Medicinal Chemistry, Drug Biology and DMPK) to facilitate drug discovery process. With this strategy, we have found several scaffolds that did not inhibit any known targets (DNA, RNA, protein synthesis, mycolic acid biosynthesis and ATP synthase). One of the scaffolds gave unprecedentedly potent (MIC=1nM) against H37Rv and MDR strains with good in vitro ADME and in vivo PK. Detail strategy and data will be described.

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장소: 제주ICC

발표코드: III-MEDLP-265

발표분야: 의약화학

발표종류: 포스터, 발표일시: 금 10:30~12:30

## Synthesis and Evaluation of Fluorine-18 Labeled Pyridopyrazine derivatives as a Potent PET Radiopharmaceutical

김희정, 김동연, \*김인종, \*박정훈, \*\*김상욱, \*허민구, \*양승대, 유국현

동국대 화학과 \*한국원자력연구원 방사선기기연구부 \*\*동국대 나노소재화학화

Wnt/ $\beta$ -catenin signaling is over expressed in various tumors, including colon cancers, lung cancers, and leukemia. Pyridopyrazine 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 pyridopyrazine derivatives for cancer imaging through Wnt/ $\beta$ -catenin signaling. 2-(4-fluorobutoxy)-3-(phenylethynyl)pyrido[3,2-b]pyrazine was synthesized in six chemical steps from commercially available 2,3-diaminopyridine and obtained in a 6% overall yield. 2-(4- $^{18}\text{F}$ fluorobutoxy)-3-(phenylethynyl)pyrido[3,2-b]pyrazine was prepared in a 20% radiochemical yield, and the radiochemical purity exceeded 97%. In vitro studies were undertaken in H460 (large cell lung cancer cells), H1299 (non-small-cell lung cancer cells), AGS (gastric adenocarcinoma cells), HepG2 (hepatocellular carcinoma cells), and MCF10A (human breast cells). An usually cellular uptake of a radio-labeled compound showed about a 2-fold higher uptake in cancer cell lines than MCF10A as a negative control cell line.

일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: III-MEDLP-266

발표분야: 의약화학

발표종류: 포스터, 발표일시: 금 10:30~12:30

## The Discovery of New 11 $\beta$ -Hydroxysteroid Dehydrogenase Type 1 Inhibitors

김태정, \*이윤희, 김남두, \*\*신영준, \*\*한창균, \*\*한동오, \*\*\*안순길

(주)유아이 \* (주)이큐스앤자루 \*\* 안국약품 (주) 중앙연구소 \*\*\* 인천대 생명과학부, (주)유아이

The glucocorticoids are a class of steroid hormones that bind to glucocorticoid receptor (GR), which is regulates or supports a variety of important cardiovascular, metabolic, immunologic, and homeostatic functions. Excess of active form of glucocorticoid induces metabolic syndromes like obesity, hypertension and insulin resistance. The 11 $\beta$ -hydroxysteroid dehydrogenase-1(11 $\beta$ -HSD1) is an enzyme that is involved in glucocorticoid regulation by catalyzing the conversion of inactive cortisone to its active form cortisol. More than 20 pharmaceutical companies have been developed the 11 $\beta$ -HSD1 inhibitors for the obesity and diabetes improvement. In this study, we proposed new scaffolds of the 11 $\beta$ -HSD1 inhibitors. Some of synthesized compounds had less than 10nM IC50 to the in vitro enzyme activity. Especially, compound EA-1398 was shown 70% inhibition to the ex vivo study in mice.

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발표코드: III-MEDLP-267

발표분야: 의약화학

발표종류: 포스터, 발표일시: 금 10:30~12:30

## Discovery of Novel B-raf Kinase Inhibitor with Potent Orally Anticancer Activity

김승용, 이윤희, 김남두, \*안순길

(주)유아이 \* (주)유아이, 인천대 생명과학부

B-raf, serine/threonine-protein kinase, is related to the Ras-Raf-MEK-ERK signal transduction. The signal pathway plays a key role in cell survival, growth and proliferation. Especially, the B-raf mutant (V600E) is found in a number of cancers, such as melanoma, ovarian, colorectal, and papillary thyroid cancers. In this study, the rational design of B-raf inhibitors were synthesized and evaluated for *in vitro* and *in vivo* assay. The compound 152 has good inhibition effect in B-raf V600E mutant type of cell-line (A375P EC<sub>50</sub>: 6nM / HT29 EC<sub>50</sub>: 5nM / COLO 205 EC<sub>50</sub>: 1nM), selectively. This compound shows a good *in vivo* efficacy in xenograft mouse model.

일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: III-MEDLP-268

발표분야: 의약화학

발표종류: 포스터, 발표일시: 금 10:30~12:30

## **New hits finding from virtual screening of the metabolic syndrome target, 11 $\beta$ -hydroxysteroid dehydrogenase-1**

**이윤호, 김남두, \*한동오, \*신영준, \*한창균, \*\*안순길**

(주)이큐스앤자루 \*안국약품(주) 중앙연구소 \*\* (주)유아이, 인천대 생명과학부

The type 2 diabetes and obesity are epidemic diseases in the world. There are many anti-diabetes and obesity targets, which have been interested from many R&D groups. The 11 $\beta$ -HSD1 converts the inactive glucocorticoid (cortisone) to active form (cortisol). The excess of cortisol is related to the metabolic syndrome, including hypertension, cardiovascular disease, dislipidemia, insulin resistance and glucose intolerance. In this study, we applied virtual screening to find new 11 $\beta$ -HSD1 inhibitors by using commercial library compounds and known X-ray structure. The virtual screening hit compounds are potent inhibition of 11 $\beta$ -HSD1 enzyme activity. Furthermore, the present the binding model of active compounds and the proposed pharmacophore would provide a useful guideline for future design of new chemical entities of 11 $\beta$ -HSD1 targeted anti-diabetic agents.

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## Econazole-derived nitroimidazoles as antitubercular agents

김수현, \*이일영, \*\*오태권, \*\*\*김필호

한국화학연구원 \*한국화학연구원 감염증치료물질연구팀 \*\*연세대 의과대학 \*\*\*한국화학연구원  
난치성질환치료제연구센터

Recently nitroimidazole series compounds get tremendous attention in the field of tuberculosis (TB) drug discovery due to their unique activities against both replicating and non-replicating Mycobacterium tuberculosis (Mtb). It has been speculated that activities against non-replicating Mtb could play a significant role in shortening the lengthy TB treatment regimen. Bicyclic nitroimidazoles such as PA-824 and OPC-67683 are currently in clinical phase II trials as a promising class of TB chemotherapy. On the other hand, antifungal agents such econazole are also known to be active against both replicating and non-replicating Mtb. During the course of studies towards discovery of novel antitubercular agents, we have explored monocyclic nitroimidazoles derived from econazole. We will present design and synthesis of monocyclic nitroimidazole analogs. Activity profiles against replicating and non-replicating Mtb will be also discussed.



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## Preparation of [ $^{68}\text{Ga}$ ]Ga-NOTA-PAMAM linker molecule for PET imaging agent

이은선, 김인종, 박정훈, \*김상욱, 허민구, 양승대, \*\*유국현

한국원자력연구원 방사선기기연구부 \*동국대 나노소재화학화 \*\*동국대 화학과

Polyamidoamine (PAMAM) dendrimers as a new class of macromolecules are known for their three-dimensional, monodispersed, highly branched with a large number of amine groups. Recently, PAMAM dendrimers have been used successfully in the field of biomedicine such as drug and gene delivery, cancer diagnosis and sensors. Hence  $^{68}\text{Ga}$  labeled NOTA-PAMAM dendrimer complex will be promising as a potent novel PET radiotracer for tumor imaging. A mixture of 2-(isothiocyanatobenzyl)-1,4,7-triazacyclononane-1,4,7-triacetic acid (SCN-Bz-NOTA) and PAMAM dendrimer in 0.1 M sodium carbonate buffer (pH 9.5) was stirred for 20 h at room temperature in the dark. NOTA-PAMAM dendrimer complex was labeled with [ $^{68}\text{Ga}$ ]GaCl<sub>3</sub> which was obtained from a  $^{68}\text{Ge}/^{68}\text{Ga}$  generator eluted with 0.1 N hydrochloric acid. We conjugated PAMAM dendrimer with SCN-Bz-NOTA to produce NOTA-PAMAM dendrimer complex using thiourea bond formation. PAMAM dendrimer has the N-terminal group with potential reactivity with the isothionate group in the NOTA derivative. [ $^{68}\text{Ga}$ ]Ga-NOTA-PAMAM dendrimer complex was rapidly labeled with  $^{68}\text{Ga}$  in 15~25% yield. The reaction mixture was purified by semi-preparative HPLC system and radiochemical purity was determined by analytical HPLC system. [ $^{68}\text{Ga}$ ]Ga-NOTA-PAMAM dendrimer complex can be quickly and easily prepare. Based on this result, we are currently developing  $^{68}\text{Ga}$  labeled nano-dendrimer composites using Fe<sub>3</sub>O<sub>4</sub> nano particles and  $^{68}\text{Ga}$  radioisotope that might be used for therapy in hyperthermia and diagnosis in the fields of PET and MRI applications.

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## Small Molecule Anticancer Agents Stabilizing G-quadruplex DNA

한수진, \*이윤성, 채정현, \*\*박현주

성신여대 화학과 \*성균관대 약학과 \*\*성균관대 약학대학

G-quadruplex structures have been often found in the promoter regions of many oncogenes and ligands which stabilize G-quadruplex could be developed as anticancer drugs. In this study, pharmacophore-based virtual screening identified three different types of heterocyclic compounds as hit compounds which stabilize G-quadruplex structures. These hit compounds showed selective PCR-arresting effects against the oligonucleotide containing c-Myc G-quadruplex sequence. Each type of compounds and its derivatives were synthesized and their activities were evaluated by PCR stop assays. Some of the newly synthesized derivatives showed increased activities in stabilizing G-quadruplex and improved cytotoxicity towards cancer cell lines.

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## Study on cardiac toxicity in the New-drug development

### 배명애

한국화학연구원 신약플랫폼기술팀

Human have been exposed to various diseases(heart disease, diabetes, cancer, etc.) as men and women lives lengthen. To treat and to prevent disease, New-drug development was performed until recently. After reported side effects of these drugs, an accurate prediction of side effects has been enforced during preclinical and early stage of New-drug development. Our research team observed the effect of 17 small molecules on heart rate measurement using the zebrafish (wild type, 72hpf) for the first time in Korea. In addition, we calculated IC<sub>50</sub> from hERG ligand binding assay result and patch clamp result of hERG transfected cell. We investigated whether there is any link between heart rate decrease in zebrafish and repolarization abnormalities.

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## Discovery of New Inhibitor for PDE3 by Virtual Screening

강남숙, \*김기영, \*이혁, \*김성환

한국화학연구원 신약플랫폼기술팀 분자설계 \*한국화학연구원 신물질연구본부

the stimulation of lipolysis by inhibiting PDE3 activity has been suggested to be a useful means for the treatment of obesity. In fact, inhibitors of PDE3 have been reported to stimulate lipolysis in adipocytes<sup>8</sup> and further study on crystal structure of human PDE3B has allowed or the design of more potent and selective PDE3 inhibitors<sup>9</sup>. In this study, the structure-based studies for PDE3 inhibitors was performed and further its enzymatic activity assay and cell-based lipolysis assay were carried out for evaluating those lipolytic activities.

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## **Prediction of dipeptidyl peptidase-IV inhibitors using Bayesian classification and fingerprint.**

김준형, 강신명, 황순희, 채종학, 강남숙

한국화학연구원 신약플랫폼기술팀 분자설계

DPP-4 is a member of a family of ubiquitous atypical serine proteases and plays a major role in glucose metabolism and a treatment for type 2 diabetes. In this study, Bayesian classification and fingerprints were used to construct highly predictive pharmacology model. In-house compounds were used for validation of this prediction model. A series of compounds with DPP2, DPP4, DPP8 and DPP9 targets were used to predict target selectivity in virtual screening. A correlation coefficient of 0.92, 0.96, 0.96 and 0.98 were obtained in predicting the activities for inhibitors of each DPP isozymes.

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## Anti-diabetic effect of a novel selective 11 $\beta$ -HSD1 inhibitor, KR-67183

김기영, \*박지선, \*\*이상달, \*\*\*정원훈, \*\*\*김희연, \*\*\*\*강남숙, \*\*\*\*\*이주연, \*\*\*\*\*배명애, \*강승규,  
\*\*\*\*\*안진희

한국화학연구원 신물질연구단 \*한국화학연구원 대사증후군치료제연구센터 \*\*한국화학연구원  
분자약리연구팀 \*\*\*한국화학연구원 약리활성연구팀 \*\*\*\*한국화학연구원 신약플랫폼기술팀 분  
자설계 \*\*\*\*\*한국화학연구원 신약플랫폼기술팀 \*\*\*\*\*한국화학연구원 대사성질환연구팀

Selective inhibitors of 11 $\beta$ -hydroxysteroid dehydrogenase type 1 (11 $\beta$ -HSD1) have considerable potential as treatment for type 2 diabetes and metabolic syndrome. In the present study, we investigated the anti-diabetic effects of KR-67183, a new 11 $\beta$ -HSD1 inhibitor, in DIO mice model. To assay cellular 11 $\beta$ -HSD1 activity, we examined by the HTRF method. KR-67183 inhibited in vitro 11 $\beta$ -HSD1 activity of human and mouse 11 $\beta$ -HSD1overexpressed cells and 3T3-L1 adipocytes. For measurement of ex vivo 11 $\beta$ -HSD1 activity, male C57Bl/6 lean mice, 12 weeks old, were orally gavaged with vehicle (0.5% CMC in H<sub>2</sub>O) or KR-67183 at 1, 5, 10 and 20 mg/kg and sacrificed 2 h post dose. KR-67183 concentration-dependently inhibited 11 $\beta$ -HSD1 activity in mouse liver and inguinal fat. Administration of KR-67183 (50 mg/kg/d, orally for 28 days) improved the glucose intolerance and insulin sensitivity and suppressed body weight gain. Moreover, KR-67183 showed good metabolic stability, and safety profile such as hERG and PXR reporter assay. We also identified the binding mode for KR-67183 for human and mouse 11 $\beta$ -HSD1. Our results demonstrate that KR-67183 improved glucose tolerance and insulin sensitivity in diabetic mice via 11 $\beta$ -HSD1 enzyme activity, and these results will provide additional support on therapeutic potential of a novel and specific 11 $\beta$ -HSD1 inhibitor in type 2 diabetes patients with obesity.

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## **In vivo evaluations and kinetic studies of F-18 labeled phosphonium salts as novel myocardial perfusion agent**

김동연, 김희정, 유국현

동국대 화학과

Despite substantial advances in the diagnosis and treatment of cardiovascular diseases, there are a few radiopharmaceuticals for diagnosis of ischemic heart diseases (IHD) using PET. F-18 labeled molecular probe for IHD is driving particular interest due to its high clinical applicability. Thus, we synthesized several kinds of F-18 labeled lipophilic phosphonium salts. Here, we evaluated the performance of F-18 labeled phosphonium salts as novel myocardial perfusion agent. We have synthesized several kinds of lipophilic phosphonium salts and have labeled no-carrier-added F-18 fluoride with the precursor, in the presence of Kryptofix-2.2.2 and  $K_2CO_3$ . For separation of F-18 labeled phosphonium salts, the last mixtures were cooled and injected onto a semi-preparative HPLC column system. Radiochemical purity was determined by analytical HPLC system. We assessed biodistribution study of F-18 labeled phosphonium salts in normal BALB/c mice ( $n = 12$ ) and dynamic micro PET study for 60 min after injecting 1 mCi of each F-18 labeled phosphonium salts. The reference compounds were synthesized in 40 - 70 % yield. Radiochemical yield was in 15~30 % and radiochemical purity was above 98% to determine by analytical HPLC system. F-18 labeled phosphonium salts showed high accumulation in the heart (over 10.00 ID %/g, at 10 min) and very rapid clearance from the blood pool and liver in normal biodistribution studies. Heart-to-liver ratio was over 1.0, 2.0, and 3.0 after 2 min, 10 min, and 20 min of each tracers injection respectively which was analyzed by time-activity curve of dynamic PET study. F-18 labeled phosphonium salts might have a potential to be utilized as a novel myocardial agent for PET in IHD and be useful for clinical cardiac PET/CT applications.

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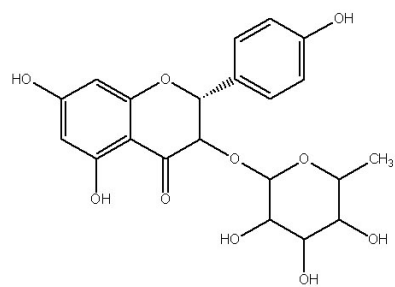
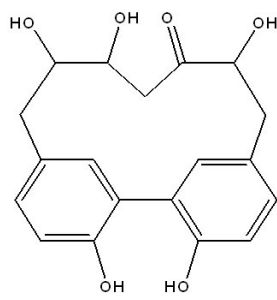
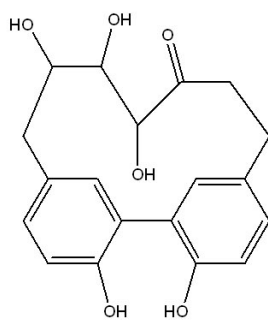
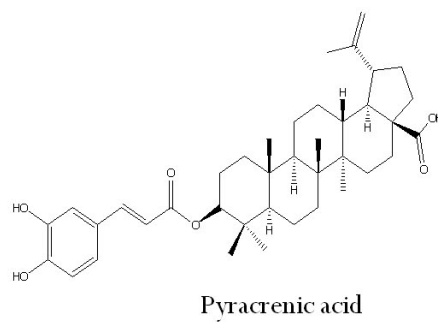
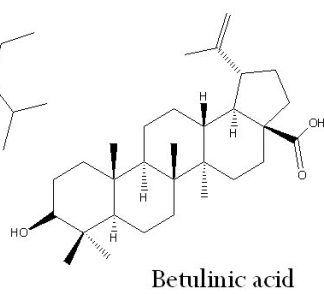
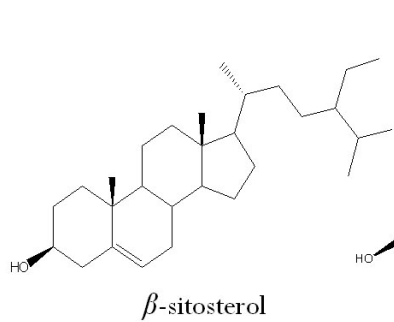
## Compounds with Elastase inhibition and free radical scavenging activities from *Carpinus coreana* Nakai

고하나, 이남호

제주대 화학과

In our continuing efforts to find biologically active compounds from plants in Jeju island, we became interested in the ethanol extract prepared from branches of *Carpinus coreana* Nakai. The repeated column chromatography of ethyl acetate-soluble fractions in this extract led to isolation six constituents such as  $\beta$ -sitosterol, betulinic acid, pyracrenic acid, carpinontriol A, carpinontriol B and kaempferol-3-O-rhamnoside. All of these compounds were isolated for the first time from this plant. Elastase inhibition and DPPH radical scavenging activities were investigated for the isolated compounds. Among these, pyracrenic acid and kaempferol-3-O-rhamnoside showed significant elastase inhibition activities with  $IC_{50}$  of 8.6  $\mu$ g/mL, 42.0  $\mu$ g/mL respectively, whose activities were comparable to a positive control oleanolic acid ( $IC_{50}$  36.1  $\mu$ g/mL). Also, pyracrenic acid showed significant DPPH radical scavenging activities with  $SC_{50}$  of 25.8  $\mu$ g/mL, more active than the positive control BHT( $SC_{50}$  78.7  $\mu$ g/mL). Based on these results, *C. coreana* branches extract could be potentially applicable as a cosmeceutical ingredient.





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## Synthesis of poly cationic polymer coupled with amino acids and $\gamma$ -aminobutyric acid as a gene delivery carrier

손상재, 배선주, 최준식

충남대 생화학과

In this study, cationic polymer of PAMAM dendrimer was synthesized with L-arginine and  $\gamma$ -aminobutyric acid (GABA) as a non-viral gene delivery vector. PAMAM G4 dendrimer was used as base polymer, which shows comparatively high transfection efficiency and low cytotoxicity than other generation. Also, dendrimer have properties of water soluble and many functional groups. GABA was used as a spacer molecule to provide hydrophobicity and flexibility. Synthesis of PAMAM G4-GABA-Arg and PAMAM G4-Arg-GABA were performed by HOBt/HBTU coupling method. To determine of characterize, we measured by  $^1\text{H-NMR}$ . Complex formation with pDNA was confirmed by agarose gel retardation assay. Additional experiments, Transfection and cytotoxicity of synthesized PAMAM G4 derivatives wae evaluated by luciferase expression assay and WST-1 assay, respectively. As a result of PAMAM G4-GABA-Arg showed enhanced transfection efficiency compared to PAMAM G4-Arg-GABA. Also, Cytotoxicity of PAMAM G4-GABA-Arg showed negligible cytotoxicity.

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## **Synthesis and Biological Evaluation of Non-acetal 12 $\beta$ (C-)-type Artemisinin derivatives for Anticancer activity.**

김현모, ricci jeremy michel, LI NA, 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, a variety of researchers have reported on the potential antitumor properties of artemisinin and its derivatives. We have special interest of its antitumor activity against human cancer cells. We synthesized novel derivatives of non-acetal deoxoartemisinin and tested in vitro anticancer activity against major human cancer cell lines. Some of synthesized deoxoartemisinin derivatives showed potent anticancer activity.

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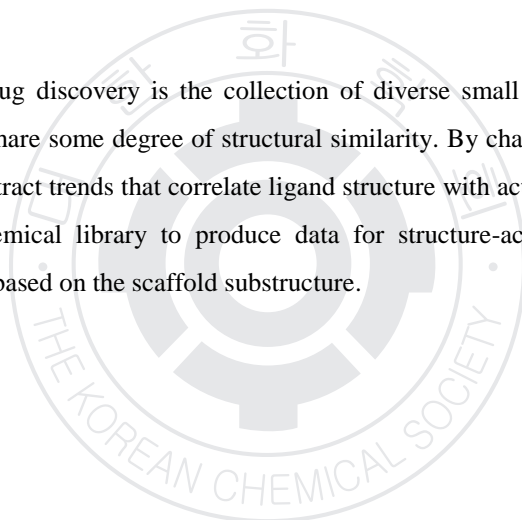
발표종류: 포스터, 발표일시: 금 10:30~12:30

## The scaffold-based library analysis

황순희, 김준형, 강신명, 김선우, 김선호, 최중권, 강남숙

한국화학연구원 신약플랫폼기술팀

A general interesting in drug discovery is the collection of diverse small molecules based on several scaffold templates, which share some degree of structural similarity. By changing the composition of the scaffold, it is possible to extract trends that correlate ligand structure with activity against a chosen target. We analyzed in-house chemical library to produce data for structure-activity analysis of medicinal chemistry project database based on the scaffold substructure.



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## The Role of Korea Chemical Bank in Hit Evaluation after HTS using Diversity Chemical Library

김선우, 우재춘, 김선호, 황순희, 채종학, 강남숙, 최중권

한국화학연구원 신약플랫폼기술팀

한국화학물은행은 산.학.연 등에서 기탁한 20 만여 종의 화합물을 관리하고 있으며 현재까지 400 개 작용점에 대한 고효율약효시험(HTS) 활용과 도출된 90 개 작용점에 대한 Hit 를 대상으로 한 선도물질화 연구를 지원하며 다양성 화합물로 구성된 독창적인 라이브러리를 운영하여 신물질개발 분야 에서 선진국과의 격차를 극복하려 한다.또한, HTS 후 도출된 Hit 평가 과정에서 Hit 화합물의 순도 및 물리화학적 물성 평가, pharmacophore 검색을 통한 SAR 자료, 작용점에 대한 최근 연구개발 동향 및 Hit 골격과의 연관성, 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 더욱 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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## Synthesis of substituted 4-pyrazol-2-benzoxazole-pyridine derivatives as novel c-Met kinase inhibitor

양전, \*이종국, \*정희정, \*하재두, \*김형래, \*조성윤

충남대 화학과 \*한국화학연구원 난치성질환치료제연구센터

Receptor tyrosine kinase (RTK) family is an attractive target for cancer therapy. C-Met kinase is a member of this family with its ligand, hepatocyte growth factor (HGF) or scatter factor (SF) which is crucial for normal mammalian development. c-Met is known to be over-expressed and mutated in a variety of human cancer types. c-Met is accountable proliferation, scattering, invasion, and metastasis of tumor cells. In an effort to search of c-met kinase inhibitors, variants of pyrazolo-benzoxazole derivatives were synthesized and evaluated toward c-met kinase inhibitory activity. Some of the compounds showed moderate activity in vitro enzymatic and cell-based assay.

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## SYNTHESIS AND ANTIMICROBIAL ACTIVITY EVALUATION OF NEW OXAZOLIDINONE DERIVATIVES

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\*\*\*KIST 케모인포매틱스연구센터

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. This 38-year innovation gap ended in 2000 with the introduction of linezolid ( marketed under the tradename Zyvox). Linezolid represents a new chemical class of oxazolidinone-containing antibacterials. Novel antibacterial oxazolidinones were synthesized and their in vitro antibacterial activities were evaluated. Most of the synthesized oxazolidinones showed good antibacterial activity against the Gram-positive and Gram-negative bacteria tested.

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## **Novel Tetrahydropyridinyl ethylamine and Piperidinyl ethylamine derivatives; their synthesis and biological activities as T-type calcium channel blocker**

이주현, \*강순방, 정낙철, \*김유승, \*\*금교창

고려대 화학과 \*KIST 생화학물질연구센터 \*\*KIST 케모인포매틱스연구센터

T-type  $\text{Ca}^{2+}$ -channel plays important role in modulating neuronal excitability on the central and peripheral neuron system, and is the essential intermediary of hormone secretion. However, hyperactivity of T-type calcium channel generates neurological disorders such as epilepsy, hypertension and neuropathic pain. On the continuous efforts on the development of T-type  $\text{Ca}^{2+}$ -channel blockers. We tried to study on the new drug active on T-type  $\text{Ca}^{2+}$  channel with good selectivity as a neuropathic pain therapy. A series of novel Tetrahydropyridinyl ethylamine and Piperidinyl ethylamine derivatives were designed and synthesized based on the 3D pharmacophore model derived from known T-type  $\text{Ca}^{2+}$ -channel blockers. The compounds were studied for the evaluation of in-vitro inhibitory activities with  $\alpha 1\text{G}$  and  $\alpha 1\text{H}$  T-type  $\text{Ca}^{2+}$  channel in FDSS assay system, and the selectivity against hERG channel, N-type, and L-type  $\text{Ca}^{2+}$ -channel. Some selected compounds were further studied PK and in-vivo activity using animal model. Therefore, we'll discuss the structure-activity relationship.



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발표종류: 포스터, 발표일시: 금 10:30~12:30

## A New Efficient Synthetic Method for 3-Iodothyronamine and its Potent Hypothermic Efficacy

전수연, 송영규, 조예현, 정찬문

연세대 화학과

Over recent years, chemically-induced hibernation has attracted much attention in fields of hibernation biology, medical science and space biology. Several compounds such as thyronamine and gaseous  $H_2S$  are shown to trigger hibernation-like state (HS) in non-hibernator mice. For instance, a single-dose administration of thyronamine elicited rapid suppression of metabolic rate, body temperature ( $T_b$ ) and heart rate, and elevated utilization of lipid over carbohydrate for metabolism in the laboratory mice. From the perspective of HS induction, 3-iodothyronamine ( $T_1AM$ ) has drawn a particular attention because it is an endogenous compound derived from a thyroid hormone  $T_4$  (thyroxine), and is found to cause little side effect or damage on neural and other critical organs even for a long-term, repeated administration.  $T_1AM$  is expected to have pharmaceutical benefits that can be applied to emergency medical care (e.g., stroke, hypoxic assault) and a long-duration spaceflight.  $T_1AM$  was synthesized by a new efficient method and its  $^1H$  and  $^{13}C$  NMR spectra are in good agreement with those previously reported. Its m.p was confirmed by DSC. The hypothermic efficacy was investigated by treating laboratory mice with  $T_1AM$  synthesized in this work.

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발표분야: 의약화학

발표종류: 포스터, 발표일시: 금 10:30~12:30

## **Facial amphipathic deoxycholic acid-modified polyethyleneimine for siRNA and plasmid delivery**

김선화

연세대 의과대학

Cardiovascular disease is one of the leading causes of morbidity and mortality in the world despite technical improvements in prevention, detection, and treatment. In recent years, there has been an increasing interest in the development of gene therapies and stem cell therapies for cardiovascular disease due to significant advances both in the understanding of the molecular mechanism of cardiovascular disease and in cell/gene delivery technology. When the cell treatment is combined with gene therapy, low-transfection efficiency is one of the major limitations. In particular, in primary cultured cells including bone-marrow-derived MSCs, most transfection techniques achieve very low efficiencies, generally no more than a few percent. Thus, preparing effective transfection methodologies is crucial to the success of gene and cell therapy for ischemic heart diseases. A class of bile acids such as deoxycholic acid has an unusual structural feature in which two to three hydrophilic hydroxyl groups face to the same direction and hydrophobic steroidal hydrocarbons orient to the opposite direction. The facially amphiphilic bile acids and their derivatives are known to interact with membrane and promote the cellular uptake of polar molecules. Herein, the facial amphipathic deoxycholic acid was conjugated to branched PEI1.8 (PEI-DA) and used in order to provide enhanced transfection efficiency of plasmid DNA and siRNA in vascular smooth muscle cells and primary cultured cells (such as MSCs), respectively.

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## Homology modeling of the metabotropic glutamate receptor subtype 1 as a target for neuropathic pain

장재완, \*배애님

과학기술연합대학원대 \*KIST 생체과학연구본부

The metabotropic glutamate receptor ( mGluR ) belongs to Class C G-protein coupled receptor ( GPCR ) and has been implicated in the diverse neurological disorders. As a drug target for the treatment of neuropathic pain, mGluR subtype 1 allosteric site has been considered important for its possible approach by various chemical substances. In an effort to develop a potent and selective mGluR1 negative allosteric inhibitor, molecular modeling studies was undertaken through one of the most state of the art techniques, homology modeling. Sequence alignment, which is the most critical part of homology modeling, was carried out with a repeated and considerable way due to low sequential identity between target and template, adopted from phylogenetically different GPCR class. After completing alignment step, 3D protein model was produced by automated model generation algorithm. Then, the validation of the model was performed by the consistency with ligand site directed mutagenesis data and small scale virtual screening. All the above procedures and corresponding results will be presented in this poster.

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## **Synthesis and binding affinity of substituted phenyl propyl piperazyl 1,2,3-triazole library as Dopamine D3/D4 receptor ligands.**

곽주명, 고훈영, 최정화, 최재이

인하대 화학과

1,2,3-Triazoles are well known heterocyclic structure as the key pharmacophore in medicinal chemistry. In continuation of our research for the discovery of potent ligands against dopamine receptor D3 or D4, the new ligands of substituted phenyl propyl piperazyl 1,2,3-triazole library is designed and synthesized by using of microwave synthesizer efficiently. Their binding affinities of constructed compounds were evaluated against dopamine receptors in vitro. And also, their structure-activity relationship will be discussed.

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## 2010-2011 Summarized report of ADME/Tox screening data in KRICT for new drug discovery

안성훈, \*송진숙, 배명애

한국화학연구원 신약플랫폼기술팀 \*충남대 약학대학

We had studied over 130 in vivo pharmacokinetic studies using SD rats, 900 in vitro pharmacokinetic studies including microsomal metabolic stability, MDCK cell permeability, CYP450 inhibition, and protein binding assay, 170 in vitro and in vivo toxicity assays for early new drug discoveries of lead and/or hit optimization. Here, we showed the summarized report of these experimental data in the view of ADME/Tox screening for early new drug discovery. Among 107 compounds we tested for estimation of bioavailability (BA) in SD rats, approximately half compounds (48%) have lower BA values than 10%. Therefore BA issues in early drug discovery stage were significant until now with or without in vitro pharmacokinetic assays. BA is calculated AUC<sub>po</sub> divided by AUC<sub>iv</sub> after dose normalization. In these studies, most compounds with high AUC<sub>po</sub> were highly related to good BA values (over 45%). With other early toxicological screening, 16-channel automated patch clamp using overexpressed hERG cells was initialized in order to evaluate the cardiac toxicity and mini-Ames test based on bacterial reversion mutation test of TA-98 and TA-100 for evaluate genetic toxicity. Our collected data may be used as the first guideline to evaluate ADME/Tox screening for early new drug discovery.

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발표종류: 포스터, 발표일시: 금 10:30~12:30

## **Dose-Independent Pharmacokinetic Profiling of a New Peroxisome Proliferator-Activated Receptor $\gamma$ agonist, KR-62980, in SD Rats and ICR Mice.**

안성훈, \*송진숙, 배명애

한국화학연구원 신약플랫폼기술팀 \*충남대 약학대학

The pharmacokinetic profiling of a novel peroxisome proliferator-activated receptor  $\gamma$  (PPAR $\gamma$ ) agonist, KR-62980 for the treatment of diabetes. The new drug candidate KR-62980 was characterized in vitro liver metabolic stability, cell permeability, plasma protein binding, and in vivo studies using Sprague-Dawley rats and ICR mice. In rat liver microsomal stability assay, KR-62980 was unstable. The metabolic half-life ( $t_{1/2}$ ) values were 11.5 ~ 15.2 min for rat and 25.8 ~ 28.8 min for human at the concentrations range of 0.1 ~ 10  $\mu$ M. In case of cell permeability, KR-62980 has a good permeability property across MDCK cell monolayers. The apparent permeability coefficient values ( $P_{app}$ ) showed a high cell permeability property of KR-62980 with the values of 20.4 ~ 30.8 ( $\times 10^{-6}$  cm/sec) at the range of 10 ~ 100  $\mu$ M. The plasma protein binding rate of KR-62980 was 89.4 % and KR-62980 was mostly bound to serum albumin (85.4 %). After intravenous administration of KR-62980 (2 mg/kg dose), the systemic clearance (CL) was 2.50 L/hr/kg and the volume of distribution at steady-state ( $V_{ss}$ ) was 9.16 L/kg. The bioavailability after oral administration was approximately 60.9 %. The dose-independent pharmacokinetics of KR-62980 after oral administration (2~10 mg/kg doses), the AUC values were 0.50, 1.02, and 3.10  $\mu$ g·hr/mL for 2, 5, and 10 mg/kg doses, respectively. In addition, in vivo pharmacokinetic profiles in ICR mice were significantly similar to those of SD rats. These data suggested that there was no significant dose-dependency in vivo studies of rats and mice even though KR-62980 may disappear rapidly from systemic circulation by liver metabolism.

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발표종류: 포스터, 발표일시: 목 10:30~12:30

## Conversion of Graphene Oxide to Reduced Graphene Oxide: Temperature Effect on the Reduction Efficiency

박경원, 문승진, 진달샘, 조영제, 이심성, 정종화

경상대 화학과

Comparative spectroscopic and microscopic analyses of the oxygen content in oxygen-containing functional groups for graphene oxide and its reduced form are reported. The graphene oxide prepared by Hummers method using graphite flakes was used as a starting material. Reduced graphene oxide was obtained through the reduction of the graphene oxide sheets with hydrazine hydrate at room temperature and 98 °C. The comparison of the oxygen content and functionality before and after the reduction of graphene oxides at different temperatures were investigated by XRD, AFM, SEM, TEM, FT-IR, XPS, and Raman spectroscopy. The reduced graphene oxides showed much larger interlayer distances (1.36 nm at room temperature and 1.08 nm at 98 °C) than those of graphene oxide (0.87 nm) and graphite (0.34 nm). According to the overall oxygen analysis data, the reduction process at 98 °C was more efficient than that of room temperature: however the epoxy- and carboxylic groups were completely removed at both temperatures.

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발표분야: 재료화학

발표종류: 포스터, 발표일시: 목 10:30~12:30

## **DNA-Mediated Anisotropic Assembly of Silver Nanoprisms and Their Diagnostic Applications**

김지영, 이재승

고려대 신소재공학부

We have synthesized the DNA-silver nanoprism conjugates (DNA-AgNPRs) and developed a thermodynamic method to control their anisotropic assemblies. The programmable anisotropic assemblies of DNA-AgNPRs have been formed simply by regulating thermodynamic conditions and demonstrated by in situ and ex situ observations. The reversible anisotropic assembly of DNA-AgNPRs exhibit distinctive optical properties and reversible cooperative binding properties. Distance-dependent optical properties associated with the reversible assembly of the silver nanoprisms have been demonstrated in the fully visible range and applied to the colorimetric detection systems for highly sensitive and selective biodiagnostic applications.



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발표분야: 재료화학

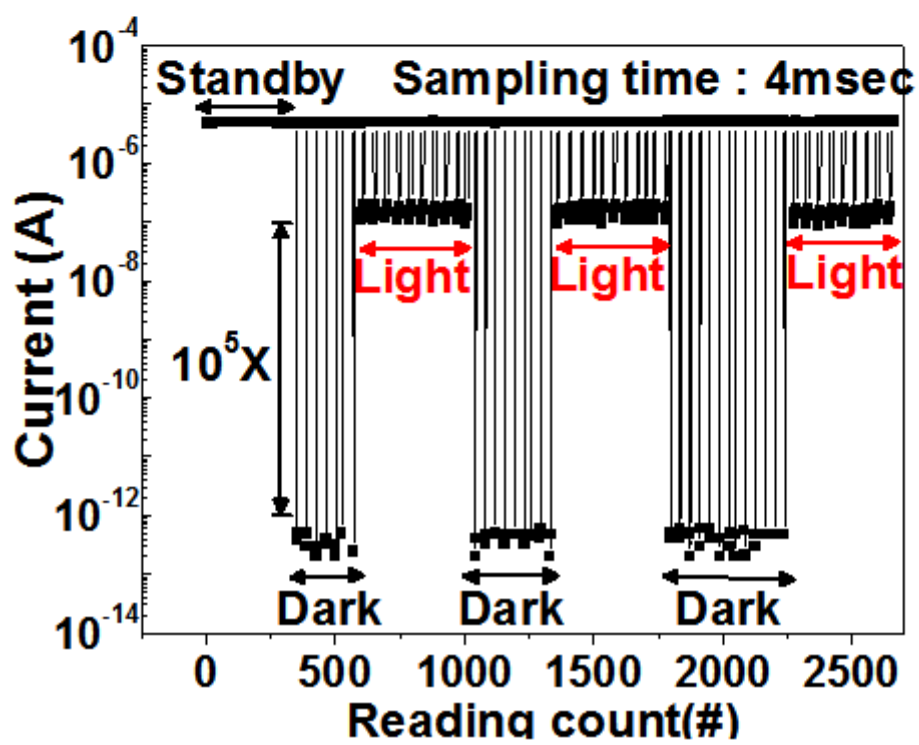
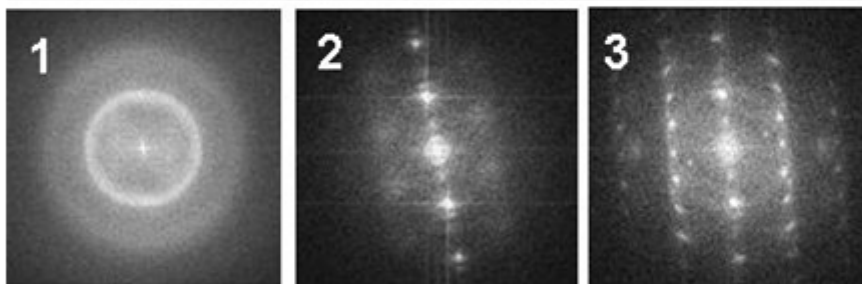
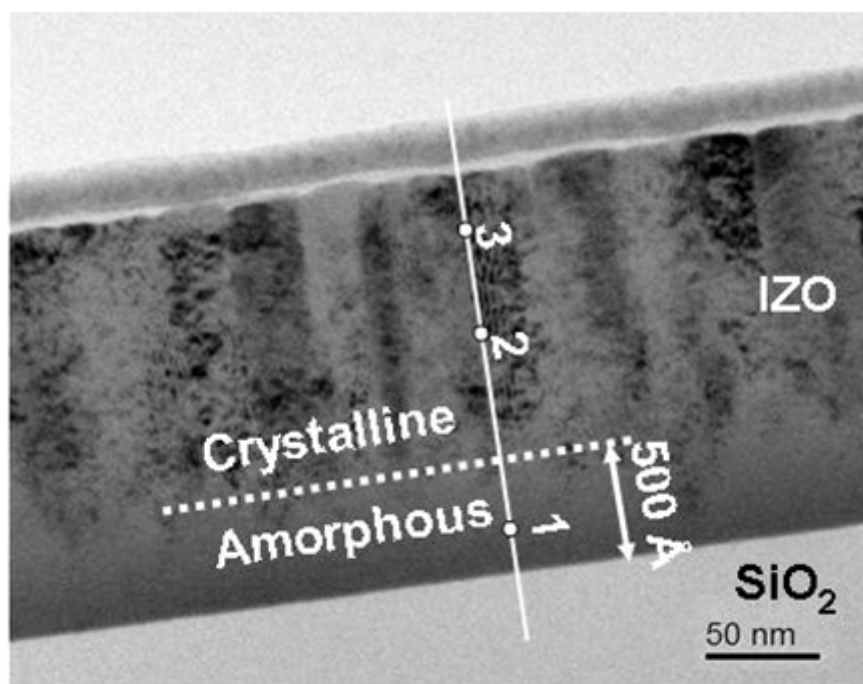
발표종류: 포스터, 발표일시: 목 10:30~12:30

## The photo-sensor device utilizing InZnO thin film transistor

박성호, 채원석, 한만소

대전대 화학과

We demonstrate the photo-sensor device based on InZnO (IZO) thin film transistor (TFT) where IZO was prepared by a radio-frequency sputtering system. Using X-ray photoelectron spectroscopy depth profile examination and high angle annular dark Field scanning TEM, it was observed that the IZO thin films with a different thickness (400, 600, 800, 1000, and 1500Å) have different crystallinity with depth profile which was changed amorphous to poly-crystal even though the composition ratio (In/Zn) of IZO with a different thickness is constant. The active channels is passivated with SiO<sub>2</sub> and photosensitivity of the device can be maximized by adjusting a reading bias. The photosensitivity (I<sub>Photo</sub>/I<sub>Dark</sub>) of the IZO TFT was significantly influenced by the device dimension and operation condition. In particular, as the active layer thickness increases, the I<sub>Photo</sub>/I<sub>Dark</sub> was increased to nearly 8 orders of magnitude, which is attributed to the current flow at back-channel of IZO TFT with crystallinity, and it exhibited slow recovery while returning to the original dark state, namely persistent photoconductivity (PPC). The adjustment of the gate voltage allows us to control the decay of PPC in the dark state. We proposed a novel sensor architecture utilizing oxide based TFT as both a switching and a photo TFTs. The operation principle proposed in this paper demonstrates the fast photo response behavior and presents the promising photo detector using oxide based TFTs.



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## Synthesis of MWCNT-AuNPs nanocomposite using functionalized MWCNT and microwave system.

이병욱, \*송재희, 이충균, 김영준

충남대 화학과 \*순천대 화학과

It is not simple to make nanocomposite of CNT-Au nanoparticles(NPs) because of aggregation and agglomeration of carbon nanotubes(CNTs). In spite of that, many studies have reported that introduced AuNPs on surface of MWCNT to improve electrical properties and find defect site of CNTs. After thiol group was introduced on surface of MWCNT, AuNPs were attached to thiol functional groups on the walls of MWCNT by using  $\beta$ -diketone. The characterization of introduced AuNPs nanocomposites has been done by using field emission transmission electron microscopy (FE-TEM), X-ray photoelectron spectroscopy checked bind interaction energy of AuNPs with thiol functional groups. The using  $\beta$ -diketone shows selective MWCNT-AuNPs nanocomposites on thermal and microwave irradiation conditions. The using functionalized MWCNT was compared with pristine MWCNT. Reaction condition was significantly reduced about 10s when microwave irradiation method was used.

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발표코드: I-MAT.P-188

발표분야: 재료화학

발표종류: 포스터, 발표일시: 목 10:30~12:30

## Synthesis of CuInSe<sub>2</sub> Nanocrystals for Their Ultraviolet Photodetecting Application

민유호, \*문건대, \*\*정운룡

연세대 신소재공학 \*연세대 신소재공학부 \*\*연세대 신소재공학과

Synthesis of semiconductor nanoparticles has been extensively studied because of their outstanding physical and chemical properties. The chalcogenide compounds which belong to III-VI and I-III-VI are one of the most attractive materials for various electronic applications. Although a large number of solution-based methods to synthesize semiconductor nanoparticles have been established, many approaches require high processing temperature, long reaction duration or specific and toxic agents. In this talk, we will provide facile synthetic routes to prepare indium selenide and copper indium diselenide nanoparticle through modified polyol process. In<sub>2</sub>Se<sub>3</sub> nanoparticle can be converted into CuInSe<sub>2</sub> nanoparticle at low reaction temperature in one hour. Thin Films device fabricated using this copper indium diselenide nanoparticle paves a way to utilizing CuInSe<sub>2</sub> nanocrystal as a ultraviolet photodetecting materials.

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발표코드: I-MAT.P-189

발표분야: 재료화학

발표종류: 포스터, 발표일시: 목 10:30~12:30

## Inorganic Nanotube Composites with Palladium Nanoparticles

**Thathan Premkumar, \*K. E. Geckeler**

*Department of Materials Science and Engineering, Gwangju Institute of Science and Technology (GIST)*

*\*Department of Materials Science and Engineering, Department of Nanobio Materials and Electronics,  
World Class University (WCU), Gwangju Institute of Science and Technology (GIST)*

Inorganic nanotubes have recently become the subject of research attention, however, their poor dispersibility in aqueous media confines drastically their applications in general and biomedical applications in particular. In this study, we prepared composites from halloysite nanotubes and palladium nanoparticles in aqueous solution by using poly-(vinylpyrrolidone) and high-speed vibration milling. It was found that the nanoparticles were deposited on the surface of the nanotubes. The hybrid materials were characterized by using FT-IR and UV-vis spectroscopy and transmission electron microscopy. The nanoparticles deposited were found to be relatively uniform in size, shape, and dimension.

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발표종류: 포스터, 발표일시: 목 10:30~12:30

## Fabrication of Core-Shell Structured Catalysts and Use in Aerobic Oxidation of Alcohols

정현민, 현다정, \*김진영, \*김용석, 이지목

금오공과대 응용화학과 \*한국화학연구원 화학소재연구단

Mesoporous silica particles are very attractive for potential applications in nano-channels, where catalytic reactions might be occurred or reactants are transported through the 1 ~ 5 nm ranged channels. The known technologies of fabrication of core-shell structures with silica-polymer particles could be applicable to form a catalyst collected in mesoporous shell. To develop metal oxide catalyst with high and size-exclusive reactivity, in this research, it is proposed that core coated with transition metal oxide nanoparticles surrounded by mesoporous shell as nano-channel cage. Ruthenium oxide core under mesoporous shell is obtained through facile three-step processes and the investigation of catalytic activity and selectivity in oxidation of secondary alcohols is performed to give high turn-over numbers and size-exclusive effects.

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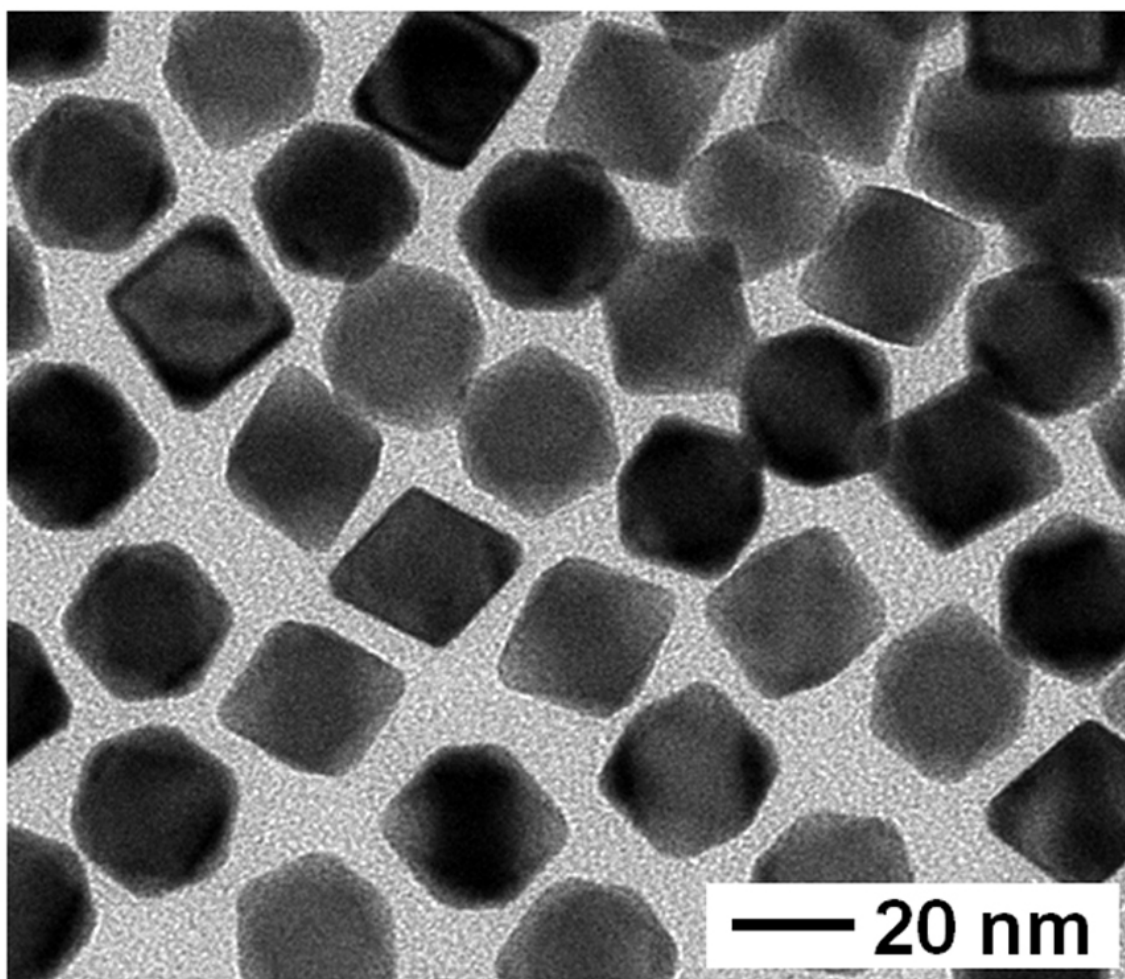
발표종류: 포스터, 발표일시: 목 10:30~12:30

## **Gold Octahedra in High Purity, and with Well-Controlled Sizes: Synthesis and Their Optical Properties**

김도엽, 박오욱

KAIST 생명화학공학과

We report a facile method for the synthesis of uniform Au octahedra with well-controlled sizes and optical properties via seed-mediated growth. Starting from single-crystal seeds of Au spheres with a uniform size, we could reproducibly obtain Au octahedra with a narrow size distribution (90%). Moreover, the edge lengths of these Au octahedra could be readily tuned in a controllable fashion from 16 to 77 nm by varying the amount of seeds, the concentration of HAuCl<sub>4</sub>, or both. We have also investigated the effects of water and poly(vinyl pyrrolidone) (PVP) in the system, as well as the reaction temperature, on the evolution of octahedral shape.





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발표종류: 포스터, 발표일시: 목 10:30~12:30

## 금속촉매를 이용한 리튬 이차전지 음극활물질용 실리콘옥사이드 나노와이어 합성

유하나, 박수진

울산과학기술대 에너지공학부

본 연구에서는 기존의 실리콘이 가지고 있는 낮은 전기 전도도와 부피팽창의 단점을 보완하기 위해 금속촉매를 이용한 리튬 이차전지 음극활물질용 실리콘 또는 실리콘옥사이드 나노와이어를 성장시키는 방법에 대해 연구하였다. 백금 또는 금과 같은 촉매물질을 실리콘 기질 위에 다양한 방법으로 코팅한 후 기상-액상-고상법 (vapor-liquid-solid growth)을 이용하여 불활성 가스의 분위기에서 공융점 이상의 온도를 가하여 실리콘 기질 위에 실리콘 (또는 실리콘옥사이드) 나노와이어를 성장시켰다. 또한 충방전 특성 평가를 통해 실리콘 또는 실리콘옥사이드 나노와이어의 전극 성능을 향상시킬 수 있음을 확인하였다. 충방전시 부피팽창이 매우 크게 발생하는 실리콘의 경우 이와 같은 방법으로 성장시킨 실리콘 나노와이어는 효과적인 방법임을 알 수 있었다.

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## Small molecule induced self-assembly of Au nanoparticles without templates

이재욱, \*주광건, \*셰드라힌아흐메드, \*\*이재범

부산대 나노융합기술학과 \*부산대 나노융합기술대학 \*\*부산대 나노메디컬공학과

Interest to one dimensional assembly of metallic nanomaterials, particularly Au nanoparticles (NPs), has grown due to the optical properties and various applications of NPs in optoelectronics, biosensors, and nano-electronics. In general, one-dimensional alignments of Au nanostructures have been accomplished by using soft or hard templates, such as polymer, DNA, anodized aluminum oxide or even molecular templates. However, difficulties of nanoscale control and remnant byproducts through unwanted chemical reactions have become limitation. In this paper, no-template assembly was successfully carried out to produce one dimensional nanochain of Au NPs through N-ethyl-N'-(dimethylaminopropyl) carbodiimide (EDC) chemistry, where carboxylates on the surface of Au NPs are activated by EDC at room temperature. EDC is a fascinating candidate for nanomaterials assembly due to its easily chemical-activating ability as well as well-known biocompatibility. Physiochemical properties of the nanochains were characterized by TEM, AFM, UV/Vis, and FT-IR spectrophotometers, as well as zeta potential. Molecular-dynamic (MD) simulations were also carried out in order to reveal the structuring mechanisms of the chains. Experimental and computational results indicate that the strong interaction between citrate-EDC-citrate and Au NPs were related with van der Waals force and the Coulomb force of functional groups, inducing delicate manipulation of the main bonding energy of self-assembly of those NPs.

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## Mechanical Properties of Multilayered Chitosan/CNT Nanocomposite Films

Sun Fangfang, \*이재범

부산대 나노융합기술학과 \*부산대 나노메디컬공학과

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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## **Formation of silica structure with the concentration changes of the silica precursor**

박지훈, 최인성

KAIST 화학과

Cysteamine, molecule that comprise an amine and a thiol group, can catalyze the formation of silica in mild conditions (i.e., at room temperature and ca. pH 7) with tetraethylorthosilicate (TEOS) which is a typical silica precursor. Our group reported that discrete silica microspheres could be formed using cysteamine, as a catalyst, and cetyltrimethylammnoium bromide (CTAB), as a insulator which is plausible role. In the previous report, we found that a simple concentration change of solvent composition resulted in the changes of the diameter of silica microspheres. Nevertheless, the concentration changes of silica precursor, although it is important condition in the process to form silica microspheres, have not been achieved yet. Here, we presented the results from the changes of the solvent composition and the concentration of silica precursor. We believe that it would be a hint to delve into the mecahnism of formation of the amorphous silica structure with the surfactant and the catalyst.

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## Synthesis and Characterization of CP-type Environmentally Friendly Explosives

강미선, 유현아, 문석식, \*김연철, 이석우

공주대 화학과 \*공주대 고분자공학과

In this study, CP-type environmentally friendly explosives were synthesized by the ligand-exchange reaction of  $[\text{Co}(\text{NH}_3)_5\text{H}_2\text{O}](\text{ClO}_4)_3$  with 5-nitrotetrazolate ( $\text{NT}^-$ ) and 5-chlorotetrazolate ( $\text{ClT}^-$ ). Positions of tetrazolate ligands in the coordination compounds were confirmed by  $^1\text{H}$  and  $^{13}\text{C}$  NMR and the configurations of  $d$ -electrons were confirmed by UV/Vis spectroscopic analyses. Thermal behaviour of compounds were investigated using DSC, and  $[\text{Co}(\text{NH}_3)_5(\text{ClT})](\text{ClO}_4)_2$  showed very strong exothermal peak around  $273^\circ\text{C}$ . After explosion, the compounds were converted to cobalt oxide and non-toxic gaseous materials. They can be used for the alternatives of the toxic explosives such as  $\text{PbN}_3$ .

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## Perhydropolysilazane을 이용한 유기-무기 복합막의 형성

강미선, 이석우

공주대 화학과

본 연구에서는 perhydropolysilazane 과 silanol terminated polydimethyl siloxane 을 혼합하여 도포 조성물을 제조하였으며, Si wafer 위에 회전도포시켜 복합막을 형성시켰다. 조성물에서 silanol 의 -OH 그룹은 silazane 과 반응하여 복합물질을 형성하였으며, 회전도포된 조성물은 가수분해에 의해 polydimethyl siloxane 을 포함하는  $\text{SiO}_2$  로 전환되었다. 고체 생성물은 원소분석, TGA, FT-IR, XRD,  $^{29}\text{Si}$  NMR 을 이용하여 특성을 규명하였으며, 조성물의 점도, 도포속도 등을 변수로 도포 두께에 대한 상관관계를 얻어 spin-on 하드마스크로의 가능성을 조사하였다.

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## **Preparation of CNT-Ag composite nanomaterials via proton beam irradiation**

송재희

순천대 화학과

Carbon nanotubes (CNT) are attractive candidates for the use as nanomaterials and nanodevices on account of their structural characteristics and promising electronic and mechanical properties. Composites of carbon nanotube with metal nanoparticles are particularly useful for use in catalysis, energy storage, and nanotechnology. Among them, CNT-Ag nanocomposites drew significant attention due to their potential applications as catalyst, and advanced materials. In this study, a new synthetic route to decorate carbon nanotube (MWCNT) with silver nanoparticles (Ag-NPs) is presented via a simple proton beam irradiation process at room temperature. Shape of the prepared silver on the surface modified MWCNT was spherical and the diameter of the silver was in the range of ~3 nm. The characterization has been done by using FE-TEM, and EDS analysis of the MWCNT/Ag composites.

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## Kinetic control of anisotropic CdTe nanocrystal production

박고운, 이성훈

서울대 화학부

Anisotropic semiconductor nanocrystals have been given a great attention as promising light-harvesting materials for the third generation photovoltaics due to their controllable bandgap in the range of UV to IR region and photost/structural stability. In order to utilize their optical and electrical properties fully, we investigated the mechanism of shape evolution of CdTe colloidal nanocrystals by the precise control of nucleation and growth kinetics. By adjusting kinetic parameters such as temperature, concentration of precursors, and injection rate, their 3-dimensional shape was drastically varied from dots, tetrapods, to branched tetrapods in a controlled manner. Their morphological uniformity and size distribution was characterized by high-resolution TEM.



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## chromatographic elution behavior of thiol end-functionalized polystyrene capped gold nanoparticles

조영진, 이원목

세종대 화학과

나노 입자들의 물리적, 화학적 특성들은 입자의 물리적 크기나 모양 분포등에 의해서 결정되고, 제한을 받는다. 최근에 다양한 분야에서 연구되고 있는 gold nanoparticles 는 여러가지 방법으로 합성되어 생화학 계통에 널리 응용되고 있다. 이러한 gold nanoparticles 은 보통 합성을 하게 되면 surfactant 로 capping 되어 용매에 분산이 되었는데, 주로 alkane thiol, aromatic thiol, amine, dialkyl disulfide 등을 사용한다. Polystyrene 은 size exclusion chromatography (SEC)뿐만 아니라 분리능이 훨씬 좋은 interaction chromatography (IC)로 분자량 별 분리가 가능하다는 것이 여러 논문을 통해 잘 알려져 있다. 때문에, thiol end-functionalized polystyrene 이 capping 된 gold nanoparticles 역시 SEC 와 IC 에서 크기별 분리가 가능할 것으로 예상 된다. 본 연구에서는, 일정한 size 의 gold nanoparticles 에 분자량이 다른 thiol end-functionalized polystyrene 을 capping 시켜서 합성 여부를 확인하고, 다양한 크로마토그래피 분리 조건 하에서, 분리거동을 관찰하였다.

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## Neutron diffraction study of $\alpha$ - and $\beta$ -polymorphs of $\text{SrTa}_2\text{O}_6$

이은혜, 김영일

영남대 화학과

Crystal structure of  $\beta$ - $\text{SrTa}_2\text{O}_6$  is reported for the first time, based on the joint Rietveld refinement of synchrotron X-ray and neutron powder diffraction patterns.  $\beta$ - $\text{SrTa}_2\text{O}_6$  crystallizes in a space group  $Pbam$  (orthorhombic, # 55) with cell parameters  $a = 12.3662(2) \text{ \AA}$ ,  $b = 12.4342(2) \text{ \AA}$ , and  $c = 3.86188(6) \text{ \AA}$ , where  $V = 593.816(2) \text{ \AA}^3$  and  $Z = 5$ . The crystal structure of  $\beta$ - $\text{SrTa}_2\text{O}_6$  consists of tetragonal tungsten bronze (TTB)-like arrays of corner-shared  $\text{TaO}_{6/2}$  octahedra, where Sr ions fill the 1-dimensional channels. For comparison,  $\alpha$ - $\text{SrTa}_2\text{O}_6$  crystallizes in a space group  $Pnma$  (orthorhombic, # 62) and has cell parameters  $a = 11.01 \text{ \AA}$ ,  $b = 7.63 \text{ \AA}$ , and  $c = 5.62 \text{ \AA}$ , with  $V = 472.5 \text{ \AA}^3$ ,  $Z = 4$ . Unlike  $\beta$ -form,  $\alpha$ - $\text{SrTa}_2\text{O}_6$  contains edge-shared dimer units of  $[\text{TaO}_{6/2}]_2$  octahedra.

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## **Facile covalent immobilization of gold nanoparticles on graphene oxide nanosheets**

**TUAN ANH PHAM, 정연태**

부경대 이미지시스템공학과

A facile approach for the preparation of novel hybrid material containing graphene and gold nanoparticles (AuNPs) is demonstrated for the first time. First, AuNPs were functionalized using 4-aminothiophenol in a single-phase system to introduce amino groups on their surface through the well-developed Au-S chemistry. Then, pristine graphite was oxidized and exfoliated to obtain graphene oxide nanosheets, which further were acylated with thionyl chloride to introduce acyl chloride groups on their surface. Subsequently, the immobilization of AuNPs on graphene surface was obtained through an amidation reaction between amino groups located on AuNPs surface and acyl chloride groups bound to GONS surface. Fourier transform infrared spectroscopy, X-ray diffraction, energy dispersive X-ray spectroscopy, ultraviolet – visible spectroscopy were used to study the changes in surface functionalities and demonstrate the successful immobilization of AuNPs on GONS surface. High resolution transmission electron microscopy and field emission scanning electronic microscopy were employed to investigate the morphologies of prepared AuNPs. Thermogravimetric analysis was used to characterize the thermal stability of the samples on heating.

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## **The preparation and surface modification of nano-sized inorganic materials**

정용주, 이철우

성신여대 화학과

One of the most probable approaches to develop novel light material with high mechanical strength is the preparation of organic-inorganic hybrid composite material using bio-inspired technology. In order to improve the stress transfer of composite material, inorganic material should have high aspect ratio, and its surface should have a strong interaction with organic material due to matrix wetting and matrix adhesion. In this study, the surface of inorganic material, such as silica and alumina, were modified to control the terminal functional group and the terminal polarity. Specifically, we modified the surface of various inorganic material using AP-TMS ((3-Aminopropyl)trimethoxysilane) and CNP-TCS ((3-Cyanopropyl)trichlorosilane). Then, the terminal functional group and polarity were controlled by additional chemical reactions. Using these surface modified inorganic materials, it is possible to control the interaction between surface-modified nano-particles.

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## Preparation and Electrochemical Characterization of Various Morphology of $\text{LiMn}_2\text{O}_4$

김주성, 모선일, \*권미숙, \*여인형

아주대 에너지시스템학부 \*동국대 화학과

Spinel  $\text{LiMn}_2\text{O}_4$  became one of the most promising candidates for rechargeable Li-ion batteries due to its multiple intrinsic advantages: structural stability, high voltage capability, low material cost, and environmentally safety. In-depth understanding and analysis of the morphology of various crystalline structures of spinel  $\text{LiMn}_2\text{O}_4$ , in conjunction with the electrochemical activities, will play a key role in improving battery performances. In this study, morphology-controlled spinel  $\text{LiMn}_2\text{O}_4$  particles with high crystallinity were successfully prepared. Various shapes of spinel  $\text{LiMn}_2\text{O}_4$  particles were synthesized from amorphous  $\text{MnO}_2$ ,  $\alpha\text{-MnO}_2$ ,  $\beta\text{-MnO}_2$  and  $\gamma\text{-MnO}_2$  as a precursor. These  $\text{MnO}_2$  were refluxed with LiI or  $\text{LiNO}_3$  to intercalate Li-ion into the lattices. Then, they were heat-treated at high temperatures to produce  $\text{LiMn}_2\text{O}_4$  with high crystallinity with maintaining their original morphologies, respectively. The crystallinity and the morphology of the materials were examined by x-ray diffraction and electron microscopic methods. Coin-type (CR2032) Li-ion rechargeable batteries were assembled with the cathode of the  $\text{LiMn}_2\text{O}_4$  and their electrochemical performances was tested and compared under various morphologies.

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## Synthesis of $\text{LiMnPO}_4$ Crystalline and Application for $\text{Li}^+$ -Cell-Cathode

**Hung-Cuong Dinh**, \*여인형, \*안지아, \*\*이종문, 모선일

아주대 에너지시스템학부 \*동국대 화학과 \*\*아주대 화학과

$\text{LiMnPO}_4$  olivine structure has become of great interest as a cathode material for rechargeable Li-ion batteries in terms of its high redox potential of  $\text{Mn}^{3+}/\text{Mn}^{2+}$  versus  $\text{Li}/\text{Li}^+$  of 4.1V, low cost of starting materials, high theoretical capacity of  $171 \text{ mAhg}^{-1}$ , and safety. However, the electrochemical performance of  $\text{LiMnPO}_4$  is poor due to the slow lithium diffusion kinetics within the grains and the low intrinsic electronic conductivity. In order to increase electrochemical characteristics, much effort has been made such as decreasing crystalline  $\text{LiMnPO}_4$  particle size (nano scale), the cation doping, carbon coated, and  $\text{LiMnPO}_4$ /carbon or polymers composite. Furthermore, various synthesis routes have been developed to overcome the weakness of  $\text{LiMnPO}_4$  such as the solid-state reaction, the sol-gel synthesis, the polyol process, and hydrothermal method. In this work,  $\text{LiMnPO}_4$  crystals nano-size and micron-size were prepared by a hydrothermal method using solution of  $\text{LiOH}$ ,  $\text{Mn}(\text{CH}_3\text{COO})_2 \cdot 4\text{H}_2\text{O}$ ,  $\text{H}_3\text{PO}_4$ , adding surfactants as factor to control size and increase specific surface of  $\text{LiMnPO}_4$  particles. The structure, morphology and electrochemical properties were examined by X-ray powder diffraction (XRD), scanning electron microscopy (SEM), impedance measurement and multichannel battery test mode.

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## ac Impedance Analysis of $V_2O_5$ and PEDOT Composite Film Cathodes

홍순기, \*유다연, \*\*여인형, 모선일

아주대 에너지시스템학부 \*아주대 자연과학부/화학과 \*\*동국대 화학과

With a nanobeam structure,  $V_2O_5$  cathode demonstrated the advantages of large surface area and high specific capacity. In this work, nanobeam  $V_2O_5$  has been embedded in a conductive polymer film during the electrochemical process of polymerization. PEDOT (Poly3,4-ethylenedioxythiophene) is one of the most successful conjugated conducting polymers with its high conductivity and the excellent environmental stability. PEDOT in the  $V_2O_5$ /PEDOT composite film can improve the electrical conductivity and the flexibility. The characteristics, together with the performance of the battery cathode, of nanobeam  $V_2O_5$ /PEDOT composite film has been investigated in depth using the methods of ac impedance measurements in the frequency range of 0.01Hz and  $10^6$ Hz at various charging/discharging states. From the ac impedance analysis at various states of charge of the battery, we can get the information about the lithium ion diffusion coefficient and the charge transfer resistance at the interfaces of electrode and electrolyte.

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## Synthesis and characterization of Double Perovskite $\text{Ba}_2\text{Bi}_{2/3}\text{TeO}_6:\text{Eu}^{3+}$ and $\text{BaBiNaTeO}_6:\text{Eu}^{3+}$ as new orange-red emitting phosphors

Nguyen Hoang Duy, \*여인형, 모선일

아주대 에너지시스템학부 \*동국대 화학과

The phosphor-coverted white light-emitting-diodes (LEDs) are the most promising light sources due to their power efficiency and lifetime. The white LEDs have been initially fabricated using blue LEDs and yellow-emitting phosphors, and red-emitting phosphor has also been introduced to improve the CRI and increase the light conversion efficiency. In this study, new orange-red emitting phosphors of double perovskite  $\text{Ba}_2\text{Bi}_{2/3}\text{TeO}_6:\text{Eu}^{3+}$  and  $\text{BaBiNaTeO}_6:\text{Eu}^{3+}$  were synthesized by a solid stated reaction. Morphology, crystal structure, and optical properties of the phosphors were examined by a scanning electron microscopy (SEM), powder-XRD and a spectrofluorometer. The phosphors  $\text{Ba}_2\text{Bi}_{2/3}\text{TeO}_6:\text{Eu}^{3+}$  and  $\text{BaBiNaTeO}_6:\text{Eu}^{3+}$  presented broad excitation bands in near UV range (350-470 nm). The emission spectra performed two peaks at about 592 nm (orange) and 615 nm (red) arising from the  $^5\text{D}_0\text{-}^7\text{F}_1$  and  $^5\text{D}_0\text{-}^7\text{F}_2$  transition of  $\text{Eu}^{3+}$ , respectively. The ratio of orange emission intensity to red emission intensity ( $I_{592\text{nm}}/I_{615\text{nm}}$ ) of  $\text{Ba}_2\text{Bi}_{2/3}\text{TeO}_6:\text{Eu}^{3+}$  is higher than that of  $\text{BaBiNaTeO}_6:\text{Eu}^{3+}$ . The emission characteristics of the  $\text{Ba}_2\text{Bi}_{2/3}\text{TeO}_6:\text{Eu}^{3+}$  and  $\text{BaBiNaTeO}_6:\text{Eu}^{3+}$  are investigated and discussed.



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## Size-controlled synthesis of ligand-protected gold nanoparticles

송지은, 이동일

연세대 화학과

Gold nanoparticles exhibit size-dependent chemical, electronic and optical properties. For the utilization of these properties in nanoelectronics, biological-sensing, and optics, it is necessary to prepare highly monodisperse gold nanoparticles protected with stabilizing ligands. We present a facile method for the synthesis of monodisperse gold particles in the range between 2 and 6 nm. Large (>4 nm) and uniform gold particles could be prepared by employing a weak reducing agent, tert-butylamine borane, in the presence of dodecanethiol and triphenylphosphine ligands. We have further developed a method to control the core size by varying the synthetic solvent composition. Uniform 2.5, 2.7, 3.4, 3.9, and 5.0 nm gold particles could be prepared in various compositions of benzene-chloroform solvent systems. This facile preparative method was successfully applied in the size-controlled synthesis of gold nanoparticles with decanethiol and hexadecanethiol.

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## Enhanced photocatalytic activity of ZnO nanoparticles modified with uniform gold nanoparticles

이재일, 이명순, 이동일

연세대 화학과

We present the preparation and photocatalytic activity of ZnO nanoparticles modified with various sized gold nanoparticles. ZnO-gold composites were prepared by anchoring bifunctional glutathione-coated monolayer-protected gold clusters (MPCs) onto ZnO. In this method, the MPC loading on ZnO can be precisely controlled without incurring size change upon anchoring. Highly monodisperse MPCs with core diameters of 1.1, 1.6, 2.7, 3.4, and 4.1nm were synthesized and used to form the ZnO-MPC composites. The photocatalytic degradation of thionine acetate was carried out with the prepared ZnO-MPC composites, which shows significant enhancement in photocatalytic activity. The composite modified with 1.1nm MPCs exhibited more than 2 times higher activity than the bare ZnO under UV irradiation. The photocatalytic activity of the composites was found to increase with increasing the size of MPCs. The origin of the size effect in the enhanced photocatalytic activity of the ZnO-MPC composites can be understood by the size-dependent capacitance of the MPCs. These results demonstrate the size effect of MPCs used in photocatalysis.

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## Synthesis and characterization of ultra-small gold clusters

박선영, 곽규주, 이동일

연세대 화학과

Ligand-protected gold clusters exhibit size-dependent chemical, electronic, and optical properties. Thiol-stabilized clusters are thermally stable and have fine structure to prevent core aggregation and decomposition. Ultra-small gold clusters protected with alkaethiols were synthesized by a one-pot synthetic method. All syntheses were carried out in air by reducing metal sources in the presence of protecting ligands in organic solvents. Chloro(triphenylphosphine)gold(I) was used as a starting material and Borane tert-butylamine complex was used as a reducing agent. The synthesized clusters have mixed ligands of triphenylphosphines and thiolates. Several organothiols were employed as the protecting ligand that includes hexanethiol, dodecanethiol, phenylethanethiol, 11-mercaptoundecanoic acid. The clusters were characterized by UV-vis absorption, fluorescence, NMR, electrochemistry, and mass spectrometry. All of the synthesized clusters exhibited similar UV-vis spectrum and fluorescence quantum yield. The electrochemical band gap of the hexanethiol-protected gold clusters was estimated to be 1.43 eV. The mass spectrometry result of the synthesized clusters suggests that the cluster consists of 37 gold atoms.

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## A Facile Synthesis of $\text{SiO}_2\text{-Fe}_2\text{O}_3$ Pillared Clay

양재훈, 한양수, \*이희숙, \*김세희

(주)나노스페이스 \* (주)세일에프에이

Porous  $\text{SiO}_2\text{-Fe}_2\text{O}_3$  pillared clay was prepared by pillaring  $\text{SiO}_2\text{-Fe}_2\text{O}_3$  nanosol particles into aluminosilicate layers. In particular,  $\text{SiO}_2\text{-Fe}_2\text{O}_3$  mixed nanosol was prepared by titrating  $\text{SiO}_2$  colloid with the suspension of iron hydroxide ( $\text{Fe}(\text{OH})_3$ ) as a base titrant. According to powder X-ray diffraction analysis, the basal spacing of  $\text{SiO}_2\text{-Fe}_2\text{O}_3$  pillared aluminosilicate (SFM) calcined at 400 °C was determined to be larger than 4.5 nm.  $\text{N}_2$  adsorption-desorption isotherm measurements showed that the BET surface area of SFMs varied from 400  $\text{m}^2/\text{g}$  to 500  $\text{m}^2/\text{g}$  depending on the amount of added  $\text{Fe}(\text{OH})_3$  in  $\text{SiO}_2$  nanosol. The prepared  $\text{SiO}_2\text{-Fe}_2\text{O}_3$  pillared clays have micropores with the size range of 0.7-1.4 nm.

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발표분야: 재료화학

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## Carbon Monoxide Removal Activity of Porous $\text{SiO}_2\text{-Fe}_2\text{O}_3$ Nanocomposites

이희숙, 김세희, \*양재훈, \*한양수

(주)세일에프에이 \* (주)나노스페이스

Porous inorganic nanocomposites were prepared by pillaring  $\text{SiO}_2\text{-Fe}_2\text{O}_3$  nanosol particles into aluminosilicate layers. In order to investigate the metal loading effect of removing carbon monoxide, various transition metals such as copper, nickel, cobalt and copper-manganese were impregnated on the porous  $\text{SiO}_2\text{-Fe}_2\text{O}_3$  nanocomposites. Metal loaded and unloaded porous nanocomposites were reduced by calcination at 400 °C under  $\text{H}_2$  gas atmosphere. According to  $\text{N}_2$  adsorption-desorption isotherm measurements, after metal-loading, BET specific surface area of porous  $\text{SiO}_2\text{-Fe}_2\text{O}_3$  nanocomposite was decreased from 450  $\text{m}^2/\text{g}$  to 350  $\text{m}^2/\text{g}$ . The reduced porous  $\text{SiO}_2\text{-Fe}_2\text{O}_3$  nanocomposite showed a higher CO-removing activity than porous  $\text{SiO}_2\text{-Fe}_2\text{O}_3$  nanocomposite.

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## **Graphitized carbon nanotube with Au nanoparticles through high temperature decomposition of sucrose in AAO template**

이명순, \*김 돈

연세대 화학과 \*부경대 화학과

The conducting carbon nanotubes decorated with Au nanoparticles were successfully prepared by the carbonization of sucrose at temperature above 973 K using Au nanoparticles(~10 nm in dia.) coated anodized aluminum oxide channels (AAO, ~80 nm dia.) as template. Within the template, sucrose was decomposed to amorphous phase carbon starting from 458 K, and the amorphous phase converted into conductive crystalline phase after annealing above 973 K for 12 h. Crystalline Au nanoparticles were stuck on the conducting carbon nanostructures, which had similar shape of pea pod. The Au particles were grown up to 50 nm from the preloaded gold nanoparticles in AAO channel template. These carbon nanostructures displayed perfect current – voltage relationship with electrical resistivity in the range 10 - 200  $\Omega\text{cm}$ .

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## The combined effect of TiO<sub>2</sub> nanotubes and nanoparticles

허라윤, \*이선흥, 주오심

KIST 청정에너지센터 \*서강대 화학공학과

TiO<sub>2</sub> nanotube has been promising as a material in solar energy conversion due to its special structure and better performance for light harvesting. The regular tubular structure provides not only charge transport path but also void. In order to remove the voids in TiO<sub>2</sub> nanotube, we prepared TiO<sub>2</sub> nanotube arrays filled and covered with TiO<sub>2</sub> nanoparticles and investigated its effect on solar cell performance of the dye sensitized solar cells(DSSC). Nanotube arrays are prepared from a titanium foil via anodization method. Using these TiO<sub>2</sub> nanotube arrays film, TiO<sub>2</sub> nanotube arrays incorporated with nanoparticles were prepared by chemical bath deposition. The details of characterization and solar cell performance with TiO<sub>2</sub> nanotube arrays filled with TiO<sub>2</sub> nanoparticles will be discussed in the presentation.

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## Optimized anodization condition of $\text{TiO}_2$ nanotube

이선흥, \*허라윤, \*주오심

서강대 화학공학과 \*KIST 청정에너지센터

In general,  $\text{TiO}_2$  nanoparticle is used as working electrode of dye-sensitized solar cells (DSSC). But high electron-diffusion-degree  $\text{TiO}_2$  nanotube shows excellent photoactivity than  $\text{TiO}_2$  nanoparticle. In this study,  $\text{TiO}_2$  nanoparticles for working electrode of DSSC were replaced by  $\text{TiO}_2$  nanotubes to increase its efficiency using the property of  $\text{TiO}_2$  nanotube.  $\text{TiO}_2$  nanotubes were synthesized by anodization of Ti plate. At this time, Nanotube's length, pore size, etc. are changed by condition of anodization. Thereabout Efficiency of DSSC is changed too. It is main object that finding optimized condition in various condition of anodization



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## **NAD<sup>+</sup> hydrogenation on Ru electrodes deposited on glassy carbon**

임지연, \*Gul Rahman, 이관영, \*주오심

고려대 화학공학과 \*Korea Institute of Science and Technology

In this study, ruthenium nanoparticles were electrodeposited on modified glassy carbon. Scanning electron microscopy (SEM), cyclic-voltammetry, chronoamperometry and linear sweep voltammetric techniques were implied to characterize RuNP deposits. The result of these studies showed that Ru nanoparticles and Ru film show significantly different catalytic activities that can be attributed to the different active surface areas of the ruthenium. The resultant RuNP/GC electrodes showed higher catalytic activity than Ru film towards hydrogenation of NAD<sup>+</sup> to NADH, indicating its potential for electro-catalytic applications.

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## Study of pH dependent, electrodeposition technique for low Pt loading

채상윤, \*Jyotiprakash B. Yadav, 김강진, \*주오심

*Department of Chemistry, Korea University, Seoul, Korea \*Clean Energy Center, Energy Division, Korea  
Institute of Science and Technology (KIST)*

Platinum has Competitive electro-catalytic activity, biocompatibility, low overpotential selectivity and environmental sustainability. It makes platinum (Pt) as a promising cathode material for water electrolysis, especially hydrogen evolution reaction. In order to reducing the cost, we fabricate Pt thin film by electrodeposition. Film morphology is controlled by adjusting pH 2 to 4.5, changing pH affect platinum complex intermediate structure, so overpotential for electrodeposition and crystal shape are changed. Furthermore, we measure the hydrogen evolution performance for each sample, sample at pH 2 shows the highest performance in our samples.

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## Observation of a Quadrupole and Higher-Order Plasmon Mode for Gold Nanorods: The effects of Roughness and Crystal Facets on Surface

홍순창, 이두리, 장희정, \*장호영, 박성호

성균관대 화학과 \*성균관대 에너지과학과

In this experiment, we prepared two types of middle aspect ratio gold nanorods for comparison of optical properties. The one was prepared in aqueous by seed mediated dropwise method in high yield (Gold nanorods in aqueous, GRA), and the other gold nanorods were synthesized by electrochemical deposition of gold into the anodized aluminum oxide (AAO) template (Gold Nanorods by template, GRT). The length was controlled by total passed charge through the cell. Size of all gold nanorods was optimized for observation of quadrupole mode. The result showed the difference of optical properties between GRA and GRT. The roughness and crystal facets on surface of gold nanorods affect optical properties.

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## Characterization of Optical Properties on Au-Ag and Pt-Ag Hollow Nanoparticles by Using the Galvanic Replacement Reaction

최윤정, 김수진, \*조성환, \*\*김상민, 박성호

성균관대 화학과 \*성균관대 에너지과학학과 \*\*성균관대 에너지과학과

In this experiment, we synthesized Au-Ag and Pt-Ag nanoparticles by using a galvanic replacement reaction with Ag nanospheres. We confirmed that both Au-Ag and Pt-Ag nanoparticles had hollow structures with the voids inside the nanoparticles through TEM images. Although a quadrupole mode which is a feature of silver nanoparticles larger than 80nm was red-shift by increasing the concentration of  $\text{Au}^{3+}$  and  $\text{Pt}^{4+}$  ions, the degree of peak shifting of Au-Ag hollow nanoparticles was much higher than that of Pt-Ag hollow nanoparticles. By comparing SEM images, we found that surfaces of Au-Ag hollow nanoparticles were different from those of Pt-Ag hollow nanoparticles. So we predict that the mechanism of generating hollow nanoparticles is different each other.

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## Surface Plasmon Coupling of Au-Ni-Ag Nanorods

이상아, \*장민선, \*\*박연주, \*\*조상현, 박성호

성균관대 화학과 \*성균관대 물리.화학융합협동과정 \*\*성균관대 에너지과학과

In this work, we demonstrated that the optical properties of AAO template synthesized Au-Ni-Ag nanorod trimers with different portion of each metal block based on surface plasmon resonance. The striped rods are composed of optically active components of Au, Ag and relatively inactive component of Ni. Transverse and longitudinal surface plasmon resonances that included higher-order modes between Au-Ni-Ag three block nanorods can be observed because free electrons in Ni block participate in coupling phenomenon. However, there was no longitudinal surface plasmon resonance coupling between the three segments as the Ni portion increased.

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## Partial hydrolysis of metal-organic porous materials

최상범, 고낙은, 심재웅, 강은영, 김자현

승실대 화학과

Partial and controlled hydrolysis of a series of iso-structural M-MOF-74 ( $M = \text{Zn}, \text{Ni}, \text{Mg}$ ) were conducted with acidic aqueous solutions. Ni-MOF-74 showed the slowest dissolution of its framework. Based on the UV-Vis spectra of the solutions and XRD patterns of the remained crystals, we could monitor the degree of hydrolysis reactions. The most interesting observation on the hydrolysis products was their type-IV nitrogen isotherms, indicating the production of mesopores. This is an easy way to create new mesopores in microporous MOFs. Moreover, this simple treatment could be applied to other types of metal-organic porous materials

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## **A metal organic framework built from Mg ions and tripodal aromatic carboxylic acids**

심재웅, 고낙은, 최상범, 오유진, 김태민, 노영수, 김자현

승실대 화학과

A porous metal-organic framework, MgTATB has been prepared by a solvothermal reaction between magnesium nitrate and H<sub>3</sub>TATB in a mixed solvent of DMF and MeOH. The framework was stable up to 500 °C based on a TGA analysis. The solvents occluded in the as-prepared crystals could be replaced with CH<sub>3</sub>CN which could be easily removed under reduced pressure. Nitrogen adsorption measurement resulted in a Type-I isotherm, and a moderate surface area: 1320 (Langmuir) and 950 m<sup>2</sup>/g (BET). However, the crystals of MgTATB diffracted X-ray very weakly, and therefore, its crystal structure could not be determined by both PXRD and single crystal X-ray analysis. We propose a model structure of MgTATB based on modeling studies and experimental observations on other two MOFs, CaTATB and SrTATB.

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## Linking the square nodes in pto-type metal organic frameworks

고낙은, 최상범, 강은영, 노경규, 노영수, 김태민, 김자현

승실대 화학과

Metal organic frameworks composed of 4 and 3-connectors can form pto net as shown in MOF-14; copper paddlewheel clusters act as square nodes and BTB linkers as triangular ones. The pto net can transform into new net when bridging ligands such as imidazolate or 4,4'-bpy link paddlewheel units; two three-dimensional porous frameworks could be synthesized by connecting Zn paddlewheel clusters in ZnBTB pto-type frameworks to give doubly interpenetrating anionic frameworks,  $\text{Zn}_3(\text{BTB})_2(\text{mIM}^-)_{3/4}(\text{mIM})_{3/4}(\text{mIM}^+)_{3/4}$  ( $\text{mIM}$  = 2-methylimidazole,  $\text{mIM}^-$  = deprotonated  $\text{mIM}$ ,  $\text{mIM}^+$  = protonated  $\text{mIM}$ , 1) and a single framework,  $\text{Zn}_3(\text{BTB})_2(4,4\text{-bpy})_{3/2}$  (2). The cation exchange in 1 with tetramethyl ammonium was confirmed by both NMR and gas adsorption measurements. The structure of 2 motivated us to make MOF-205,  $\text{Zn}_4\text{O}(\text{BTB})_{4/3}(\text{NDC})$  following it-d net.



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## Syntheses of Zn(O,S) thin films in acidic aqueous solution

이예지, 정덕영

성균관대 화학과

Zinc oxy-sulfide [Zn(O,S)] thin film is a promising alternative as a Cd-free buffer layer in Cu(In,Ga)Se<sub>2</sub> (CIGS) solar cell. The Zn(O,S) films on glass substrates were prepared in the acidic aqueous solution, including zinc acetate, thioacetamide (TAA), hydrazine and trisodium citrate, where hydrazine and trisodium citrate were used as coordinating ligands. The as-deposited and annealed films were characterized by scanning electron microscopy, electron probe X-ray micro analysis (EPMA), Raman spectroscopy, X-ray diffraction, UV/Vis spectroscopy. The Zn(O,S) thin films showed good uniformity overall areas and the large band gap of about 3.5 eV. For electrical properties of Zn(O,S) thin films deposited on the CIGS were confirmed to p-n junction by current-voltage characteristics.

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## Catalytic Activity of Platinum Nanoparticles Immobilized on Layered Double Hydroxide Nanosheets

김하나, \*이종현, 정덕영

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Platinum nanoparticles (Pt-NPs) immobilized on layered double hydroxide (LDH) nanosheets were successfully prepared. Pt-NPs with diameters between 2 and 5 nm were adsorbed uniformly on to the LDH nanosheets. The catalytic activity were measured for hydrogenation reaction of p-nitrophenol and monitored by using UV-Vis spectrophotometer at room temperature. Pt-NPs on LDH could be used as catalysts repeatedly for several cycles thanks to stabilization on LDH surface. The transmission electron microscopy showed that Pt-NPs were adsorbed strongly on LDH nanosheets without aggregation even after recycle processes. On the contrary, Pt-NPs without LDH were aggregated just after the first recycle which decreased catalytic activity. Collection of the Pt-NPs and LDH catalyst after use was facile through filtration instead of the time consuming centrifugation steps. Pt-NPs on LDH have an outstanding advantage in recycle for several times, their catalytic activity was maintained over 90 percents even though there was small loss of Pt contents.

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## Ultra-Sound Induced Rapid Intercalation of Biselenite in Layered Double Hydroxides

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By using a facile ultrasonic treatment in ethanol, the de-intercalation of carbonate ( $\text{CO}_3^{2-}$ ) ions from MgAl-layered double hydroxides (LDHs) ( $\text{Mg}/\text{Al} = 2$ ) both on monolayer films and powdery samples was investigated at atmospheric conditions. We used ethanol as a reaction medium and the selenous acid as a precursor to incorporate into the interlayer gallery. Under 0.5 M of selenous acid ( $\text{H}_2\text{SeO}_3$ ) concentration and 30 minutes of reaction time for powdery LDHs, and 0.1 M and 5 minutes for the thin film LDHs, the carbonate ions were successfully exchanged with biselenite ( $\text{HSeO}_3^-$ ) ions. The electron microscopy clearly indicated that the morphologies of the original LDH particles were preserved after the reaction, even though the ultra-sound was continuously applied up to 2 hours of reaction time. The results of XRD, FT-IR and Raman scattering strongly suggested that the cyclic dimer of biselenite ions are incorporated into the gallery space of LDHs, vertically arranged to the horizontal axes of MgAl-LDH layers.

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## Electrochemical deposition of $\text{Cu}_2\text{ZnSnS}_4$ thin films for photovoltaic cell

김지현

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 formed by electro-deposition using ternary metal salt solution, tartaric acid and tri-sodium citrate at room temperature and sulfurized in elemental sulfur vapor ambient for 1h blowing Argon gas. Stoichiometric and morphological properties of the as-deposited films and samples after heat treatment were characterized by scanning electron microscopy (SEM), energy-dispersive X-ray spectroscopy (EDS), and X-ray diffraction (XRD). The thickness and metal ratio of the optimized CZTS absorber layers was 1 micrometer and  $\text{Cu} : \text{Zn} : \text{Sn} : \text{S} = 2 : 1 : 1 : 4$ . We also investigated electrical characteristic by using I-V measurement.

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## Superlattice Structure $\text{Cu}_{1-x}\text{S}$ , $\text{Ge}_{1-x}\text{Sb}_x\text{Te}$ , and $\text{Ge}_{1-x}\text{Bi}_x\text{Te}$ Nanowires

김한성, 정찬수, 장소영, 박정희, \*안재평

고려대 소재화학과 \*KIST 산업화지원센터

Single-crystalline wurtzite CdS nanowires (NWs) underwent gas-phase substitution to form unique superlattice cubic  $\text{Cu}_{1.8}\text{S}$  (digenite) and hexagonal  $\text{Cu}_2\text{S}$  (chalcocite) structures, using thermal evaporation of  $\text{CuCl}_2$  at 500~600 °C. The  $\text{Cu}_{1.8}\text{S}$  NWs consisted of superlattices along the direction, with controlled growth direction ([110], [211], [100], [111]) and superlattice periods of five (111) planes (1.6 nm) and six (111) planes (1.9 nm); as the temperature decreased, the growth direction evolved from [100] to the higher surface-energy [110] or [112] directions, with longer superlattice periods. The  $\text{Cu}_2\text{S}$  NWs also exhibited a superlattice along the [0001] growth direction, with a periodicity of eight (0002) planes (2.7 nm), and could be irreversibly converted into superlattice  $\text{Cu}_{1.8}\text{S}$  (six (111) planes; 1.9 nm) by electron-beam irradiation of transmission electron microscopy. We successfully synthesized ferroelectric  $\text{Ge}_{1-x}\text{Sb}_x\text{Te}$  and  $\text{Ge}_{1-x}\text{Bi}_x\text{Te}$  NWs by vapor transport method. The doping concentration of Sb and Bi was controlled in the range of 0-50 % using the growth condition. The undoped GeTe NWs consisted of single-crystalline rhombohedral structures with the [001] or [021] growth direction. Low-concentration (

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## Reverse micelle법을 이용한 $\text{CaMgSi}_2\text{O}_6:\text{Eu}^{2+}$ 청색 형광체의 합성 및 투명 형광막 특성 연구

장미, \*최성호, \*\*정하균

고려대 신소재공학과 \*한국화학연구원 소자재료연구센터 \*\*한국화학연구원 화학소재연구본부

대형화 제품에서의 가격경쟁력 및 3 차원 이미지 구현에 유리한 특성을 바탕으로 최근에 플라즈마 디스플레이(PDP)가 다시 주목 받고 있다. 이러한 최근의 기능성 디스플레이를 구현하기 위해서 형광체의 요구특성도 변하고 있다. 형광체 입자가 나노 크기로 작아지면 벌크 형태의 형광체에 비해 도포되는 면적이 커지기 때문에 입자 밀도가 증가해 효율적으로 발광에 기여할 수 있지만, 비발광 전이를 유도하는 표면 특성의 효율적인 제어가 요구된다. 또한 불규칙한 입자보다는 균일한 입도분포(특히 구형)를 가지는 형광체를 사용함으로써 방출 되는 빛의 산란이 적고 화면의 밝기와 해상도를 증가시킬 수 있다. 본 실험에서는 역미셀(Reverse micelle) 방법을 이용해 청색발광  $\text{CaMgSi}_2\text{O}_6:\text{Eu}^{2+}$  나노입자를 합성하였다. X-ray 회절법을 이용해 단일상 구조를 확인하였으며, 진공자외선 여기 하에 445nm 부근의 청색 발광 스펙트럼을 보였다. 합성된 형광체는 0.76ms 의 짧은 잔광 시간을 가졌으며 200nm 의 입자 크기 및 morphology 를 관찰할 수 있었다. 또한  $\text{CaMgSi}_2\text{O}_6:\text{Eu}^{2+}$  나노형광체를 2-Methoxyethanol 에 분산시키고 스핀 코팅법을 이용하여 투명유리기판에 형광막을 형성하였다. 완성된 형광막의 투과도 및 Xe/Ne 가스 방전 하에서의 발광 특성을 확인하였다.

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## Optimization of partially dyed-TiO<sub>2</sub> compositions for printable photoanodes in DSSCs

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염료감응 태양전지 (Dye-Sensitized Solar Cells, DSSCs)의 기본 개념은 오래 전부터 알려져 있었으나, DSSCs 가 많은 관심을 끌게 된 계기는 약 20 년 전 다공성 나노 결정성 TiO<sub>2</sub> 를 이용하여 약 7%의 광전환효율이 보고된 이후이다. 이후 많은 실험실에서 DSSCs 의 효율을 증가시키기 위한 연구가 수행되어 현재에는 photon-to-current efficiency 가 약 11 %에 도달하였다. 이에 따라, 다양한 응용분야에 DSSCs 를 접목하기 위해 flexible 한 기판위에 저온소결을 통해 광전극을 제조하는 DSSCs 분야에도 많은 연구가 진행되고 있다. 그러나, flexible 광전극 기판을 사용하는 DSSCs 가 시장에서 성공적으로 론칭하기 위해서는 R2R 연속공정과 같은 대량생산을 통하여 DSSCs 제조 원가를 혁신적으로 감소시키는 연구가 필수적이다. 이를 위해서는 TiO<sub>2</sub> 의 저온 sintering 과정과 dye-adsorption 시간 단축이 필수 불가결하다. 본 연구에서는 저온에서 제조된 TiO<sub>2</sub> film 을 compression 한 후에 dye 를 흡착시키는 공정 대신, 기 dye 가 부분적으로 흡착된 TiO<sub>2</sub> 를 compression 하는 방법을 통하여 저온 공정이 가능하고 dye 흡착 시간이 생략된 새로운 방법을 이용하였다. 그리고 dyed-TiO<sub>2</sub> 의 size, dye 흡착량, pressure 등의 실험 결정 매개 변수를 변화시켜 524,288(2<sup>19</sup>) 개의 가짓수를 실험대상군으로 하였다. 이러한 수십만 개의 DSSCs 를 개별 제작하여 변수에 따른 성능을 비교하는 사실상 불가능하다. 그리하여 우리는 Heuristics 기법을 통하여 매개변수의 조합을 최적화함으로써 R2R 연속공정에 적용 가능한 TiO<sub>2</sub> 조성을 확립하는 연구를 수행하였다.

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## **Barrier layer effect on the electron transfer of the dye-sensitized solar cells based on TiO<sub>2</sub> nanotube arrays**

이혜연, 서정쌍

서울대 화학부

We have studied the effect of the barrier layer to the electron transfer of the dye-sensitized solar cells (DSSCs) based on TiO<sub>2</sub> nanotube arrays. The barrier layer of TiO<sub>2</sub> nanotubes, corresponding to the bottom surface of the detached TiO<sub>2</sub> nanotube films, was ion milled to reduce its thickness. The energy conversion efficiencies, measured by a back-side-illumination, of DSSCs based on the TiO<sub>2</sub> nanotube films whose barrier layers were ion-milled for 0, 10, 20, and 30 min were 1.2, 1.4, 1.6 and 1.7%, respectively. The conversion efficiency increased significantly with reducing the thickness of the barrier layer, without opening the bottom tips. The improvement of the conversion efficiency was mainly due to the improvement of the electron transfer efficiency with reducing the thickness of the barrier layer. It was concluded that the electron transfer is hindered seriously by the barrier layer.



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## Pseudocapacitance Behaviors of Nanostructured Manganese Oxides Synthesized by Room Temperature Solution Reaction

성다영, \*김인영, \*\*김태우, \*황성주

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The nanostructured  $\delta$ -,  $\gamma$ -, and  $\alpha$ -MnO<sub>2</sub> materials are synthesized at room temperature via one-pot oxidation reaction of divalent manganese compounds such as MnO, MnCO<sub>3</sub>, and MnSO<sub>4</sub>. From the N<sub>2</sub> adsorption-desorption isotherm measurements, the obtained manganese oxide nanostructures possess large surface area of ~50-120 m<sup>2</sup>/g. Also, the Mn K-edge X-ray absorption measurements demonstrate that all the manganese ions in the present materials are stabilized in octahedral symmetry with the mixed oxidation state of Mn<sup>3+</sup>/Mn<sup>4+</sup>. All of the nanostructured manganese oxides exhibit pseudocapacitance behaviors with large specific capacitance and good capacitance retention, highlighting their promising functionality as a supercapacitor electrode. Among the materials under investigation, the  $\delta$ -MnO<sub>2</sub> 2D nanoplates show the largest electrode activity with the best cyclability, clearly demonstrating the merit of layered structure in electrode application.

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## Self-Assembly of Reduced Graphene Oxide/Layered $\text{MnO}_2$ Nanosheets with Lithium Cations

이유리, 이경민, 김인영, \*김태우, 황성주

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Porous nanocomposites of Li-reduced graphene oxide (RGO)-layered manganate nanosheets are synthesized via the co-flocculation of exfoliated  $\text{MnO}_2$  and RGO nanosheets with lithium cations. According to X-ray diffraction and electron microscopic analyses, both the  $\text{MnO}_2$  and RGO nanosheets are porously restacked with lithium ions, resulting in the formation of porous structure by the house-of-cards type stacking of layered crystallites. Mn K-edge X-ray absorption spectroscopy clearly demonstrates that manganese ions in the reassembled materials were stabilized in octahedral symmetry with the mixed oxidation state of  $\text{Mn}^{3+}/\text{Mn}^{4+}$ . The present reassembled manganates with RGO show large specific capacitances of ~140-160 F/g in  $0.5 \text{ mA/cm}^2$ . This study provides strong evidence for the effectiveness of exfoliation-reassembling method in enhancing the capacitance performance of layered metal oxides.

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## **Synthesis of highly crystalline mesoporous transition metal oxides using laboratory made diblock copolymer as structure directing agent and their application to photocatalyst**

황종국

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Highly crystalline and thermally stable mesoporous titanium oxide and niobium oxide with uniform pores have been synthesized by using laboratory made poly(ethylene oxide)-b-polystyrene(PEO-b-PS) diblock copolymers as structure directing agent. The amphiphilic diblock copolymers with various molecular weights were prepared through simple synthetic method called atom transfer radical polymerization (ATRP). This method can be easily applicable to researchers without any experiences in polymer synthesis. Pore size of transition metal oxides can be also easily controlled by changing the molecular weight of structure directing agent, PEO-b-PS. The photocatalytic activity of prepared TiO<sub>2</sub> (CASH-TiO<sub>2</sub>) for water splitting and Methylene Blue degradation was studied and the TiO<sub>2</sub> (P123-TiO<sub>2</sub>) templated by commercial triblock copolymer Pluronic P123 was used for comparison. The photocatalytic activity of CASH-TiO<sub>2</sub> was about 2 times higher than that of P123-TiO<sub>2</sub> in both hydrogen evolution and MB degradation. Though CASH-TiO<sub>2</sub> has smaller surface area than the P123-TiO<sub>2</sub>, it exhibited high activity due to efficient charge transfer resulting from high crystallinity of mesostructured walls.

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## Cocatalyst-Free Photocatalysts of CdS Quantum Dots-Layered Titanate Nanohybrids for Enhanced H<sub>2</sub> Generation

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CdS quantum dots (QDs)-layered titanate nanohybrids were synthesized in terms of an electrostatic attraction between positively charged CdS QDs and negatively charged exfoliated titanate nanosheets. A combinatorial analysis of transmission electron microscopy, selected area electron diffraction, and powder X-ray diffraction clearly demonstrates the formation of CdS-layered titanate nanohybrids. According to the UV-vis spectroscopy, the hybridization of CdS QD and exfoliated titanate nanosheets causes a distinct narrowing of bandgap energy in comparison to bare materials from 2.9 eV (CdS QDs) to 2.5 eV (CdS-layered titanate nanohybrids). Also, there occurs an efficient electron transfer from CdS QDs to layered titanate, as evidenced by photoluminescence spectroscopy. Moreover, N<sub>2</sub> adsorption-desorption isotherm analysis indicates that the CdS-layered titanate nanohybrids have 100 times larger surface area than the pristine layered titanate. On the basis of the obtained results, the present CdS-layered titanate nanohybrids show high photocatalytic activity for the H<sub>2</sub> production under visible light illumination without any cocatalysts.

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## **Influence of Copper Oxide on Supercapacitive Properties of Activated Carbon Nanotubes**

김대원, 박수진

인하대 화학과

In this work, we synthesized copper oxide (CuO)-doped activated multi-walled carbon nanotubes (CuO-ACNTs) to evaluate their potential applicability as supercapacitor electrodes. The ACNTs were prepared by chemical activation methods with KOH, and then a series of CuO-ACNTs were prepared by chemical deposition with different CuO ratios. The textural properties of the CuO-ACNTs were investigated by N<sub>2</sub>/77 K adsorption isotherms using Brunauer-Emmett-Teller (BET) equation and BJH method. The surface morphology was characterized by scanning electron microscope (SEM) and transmission electron microscopy (TEM). The electrochemical performance of CuO-ACNTs was determined by cyclic voltammetry (CV) and galvanostatic charge/discharge characteristics in 6 M KOH electrolyte. As a result, the specific capacitance of CuO-ACNTs was improved with increasing CuO ratio, indicating that their improved capacitance was attributed to pseudo-capacitive effect of CuO introduced onto ACNTs.

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## In-Depth Electrical Test Analysis of the Influence of Particles Size and Crystallinity of $\text{LiV}_3\text{O}_8$ on the Battery Performance of $\text{LiV}_3\text{O}_8$ Based Cathodes

Quang-thao Ta, \*여인형, 모선일

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The lithium trivanadate ( $\text{LiV}_3\text{O}_8$ ) has been receiving attentions as a candidate material with a feasibility of providing a high capacity structurally safe and environmental friendly lithium rechargeable battery. However, it has been suffered by its low cyclic stability which are critical disadvantages to be a good battery electrode material. In this work, to investigate these disadvantages and then eventually improve the battery performance, both nano-sized and micron-sized crystalline  $\text{LiV}_3\text{O}_8$  particles without carbon/polymer coating have been intensively investigated using in-depth analytical test analysis, in conjunction with the X-ray diffraction spectroscopy, SEM and FTIR spectra analysis. For the understanding of the in-depth electrical test analysis, correlation among CV, AC impedance, battery charge/discharge and GITT are studied together with extraction of the electrochemical parameters, such as chemical diffusion constant and crystal phase changes, during different states of lithium intercalation and de-intercalation.

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## **Influence of Surface Modified Multi-Walled Carbon Nanotubes on Mechanical Properties of Epoxy Composites**

김대원, 박수진

인하대 화학과

In this work, we prepared the surface modified multi-walled carbon nanotubes (MWNTs) in order to improve mechanical properties of epoxy composites and MWNTs were surface modified using nitric acid and hydrofluoric acid. The effects of surface modified MWNTs on mechanical properties of diglycidyl ether of bisphenol-A (DGEBA)/MWNTs composites were investigated with fracture toughness and impact tests. Their fractured surfaces were examined with a scanning electron microscope (SEM) to investigate the phase morphologies of the composites. From the results, the mechanical properties of the DGEBA were improved with the addition of surface modified MWNTs, due to strong intermolecular interactions between DGEBA and MWNTs. The SEM micrographs showed that MWNTs particle-DGEBA debonding had occurred to prevent deformation and crack propagation in the DGEBA/MWNTs composites.

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## 초상자성 $\text{MnFe}_2\text{O}_4$ & $\text{ZnFe}_2\text{O}_4$ 나노입자 합성

남준식, 정종형, 정진승

강릉대 화학과

최근, 자성 나노입자의 초상자성 특성을 이용해 촉매, 생명공학/생의학, 자기공명구조(MRI), 자성 유동체, 환경화학적 개선 등 다양한 분야에 많이 응용되고 있다. 특히 나노·바이오 융합연구를 위해서는 수용성이며 자화값이 큰 초상자성 특성을 갖는 나노입자가 필요하다. 본 연구에서는 초상자성 특성을 갖는  $\text{MnFe}_2\text{O}_4$  와  $\text{ZnFe}_2\text{O}_4$  를 EG/DEG 양 조절을 통해 다양한 크기로 합성하였다. 합성된  $\text{MnFe}_2\text{O}_4$  와  $\text{ZnFe}_2\text{O}_4$  는 primary 나노결정의 크기가 강자성 특성을 갖는 단자구 임계 크기보다 작기 때문에 secondary  $\text{MnFe}_2\text{O}_4$  와  $\text{ZnFe}_2\text{O}_4$  의 크기가 수백나노의 크기를 가져도 상자성 특성을 나타내게 된다. 다양한 크기로 합성된  $\text{MnFe}_2\text{O}_4$  및  $\text{ZnFe}_2\text{O}_4$  의 구조를 SEM, TEM, XRD, EDX, IR 을 이용해 측정하였다.

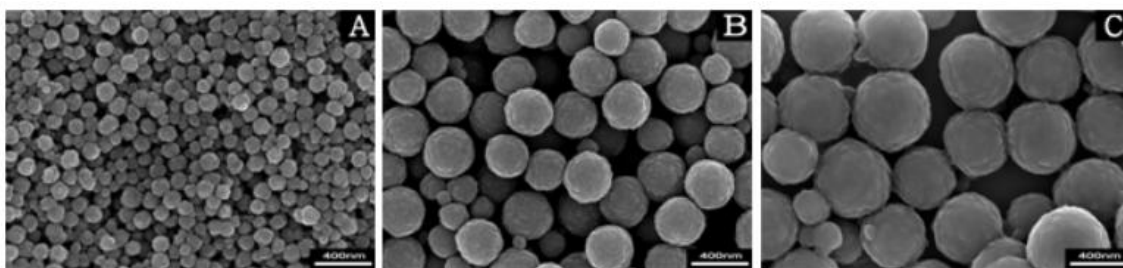


Figure. SEM Image A) 100nm , B) 300nm, C) 500nm  $\text{MnFe}_2\text{O}_4$



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## Preparation of Micron-sized Silica Particles by Colloid Aggregation Method

강영주, 윤주영, 양재훈, 한양수

(주)나노스페이스

Micron-sized  $\text{SiO}_2$  particles with the size of 3.0~6.0  $\mu\text{m}$  are prepared by colloid aggregation method, which involves polymerization of urea with formaldehyde in the presence of colloidal silica. During the aggregation process, the urea and formaldehyde gradually consumed to form melamine-silica hybrid particles. Upon heating at 500  $^{\circ}\text{C}$ , monodispersed and porous silica particle with micron-size are obtained. In the present study, particle size and its distribution could be controlled by varying the synthetic parameters such as concentration of colloid silica, urea and HCl. In addition, the mixing order of colloid silica, urea and HCl have an effect on the particle size and its distribution. It is found that the decrease in solution pH resulted in the decrease of average particle size and the increase of monodispersity of silica particles. The particle characteristics including shape, size, size distribution, and porous texture will be discussed on the basis of XRD, SEM, TEM, and nitrogen adsorption-desorption isotherm analyses.

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## Preparation of New Zinc Pyrithione-Clay Nanocomposite

강영주, 윤주영, 한양수

(주)나노스페이스

Zinc pyrithione is known for its use in treating dandruff and seborrheic dermatitis. It is the active ingredient in several anti-dandruff shampoos and preservatives. However, it has very low solubility and poor dispersion property in water and organic solvents. In the present study, a novel zinc pyrithione-clay nanocomposite was prepared by solid state reaction method to improve the solubility in aqueous and organic solvents. At first, micron-sized zinc pyrithione was mixed with alkylamines, and then melted to obtain clear liquid, followed by mixing and grinding with expandable clay, finally resulted in the zinc pyrithione-clay nanocomposite. The zinc pyrithione-clay nanocomposite shows remarkable swelling and dispersion property in organic solvents like benzene.

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## Intercalative Nanocomposite between Cocamide DEA and Swellable Clay by Solid State Process

최민아, 윤주영, \*이지호, \*\*이남호, 한양수

(주)나노스페이스 \*인하대 화학과 \*\*제주대 화학과

Intercalative compound of cocamide DEA (CDEA) and clay minerals have been prepared by solution and solid state intercalation processes. In the solid state intercalation process, the CDEA molecules have paraffin-like double layer arrangement between the silicate layers with the expansion of the basal spacing as large as 44 Å. Weak van der Waals interaction plays an important role in the formation of organic-inorganic nanocomposite. Upon washing, however, the interlayered CDEA molecules are mostly leached out when the interlayer cations are Na<sup>+</sup> or Ca<sup>2+</sup>. Even though the basal spacings of the CDEA-protonated clays complexes also decrease largely after washing, they exhibit distinct diffraction profiles at 13.5 Å, which can be assigned to the monolayer CDEA arrangement between the silicate layers. It is sure that the solid state intercalation reaction between protonated clays and CDEA seems to be occurred by an intralayer acid-base complexation between interlayered proton (H<sup>+</sup>) and basic ethanolamine function groups.

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## A Simple Route to Intercalative Organo-Clay Nanocomposites

도보영, 윤주영, \*정철연, \*\*이남호, 한양수

(주)나노스페이스 \*제주대 생명공학 \*\*제주대 화학과

Intercalative layered nanocomposites of expandable clays (natural montmorillonite and synthetic hectorite) and alkylammonium molecules are prepared. In particular, a simple solid state intercalation route could be applied successfully to the preparation of layered nanocomposite. In the solid state process, alkylammonium molecules have a paraffin-like arrangement between silicate layers with the expansion of basal spacing as large as 40 Å. Additional weak van der Waals interaction plays an important role in the formation of paraffin-like stacking structure. Upon washing, some interlayered molecules adsorbed excessively are leached out, resulted in the decrease of basal spacing. The layer stacking structure of organo-clay composites formed by solid state process are discussed in detail according to the kind of clay, organic templates, template loading level, etc.

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## Intercalative Nanocomposite for Essential Oil Delivery Support

도보영, \*정철연, \*\*이남호, 한양수

(주)나노스페이스 \*제주대 생명공학 \*\*제주대 화학과

Layered nanocomposites between alkylammonium surfactants and clay minerals have been applied as delivery support for hydrophobic essential oils such as alpha-pinene, camphene, etc. Inclusion of essential oils with high volatility and poor water solubility could be achieved through the van der Waals interaction between hydrophobic oil molecules and surfactant chain. In particular, solid state intercalative process has been successfully applied in the preparation of intercalative nanocomposite including highly non-polar oil molecules. Hydrophobically modified interlayer spaces of clay act as sorption site and stabilize unstable active ingredients.

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## Synthesis of uniform core-shell silica nanoparticles with various mesoporous shell structures

김정호, 김민식, \*Nitin Chaudhari, \*\*chaudhari kiran, \*\*\*양대수, \*송민영, \*최혁수, \*김윤경, 권선영, \*박진술, \*최은지, 유종성

고려대 신소재화학학과 \*고려대 소재화학과 \*\*고려대 소재화학 \*\*\*고려대 신소재화학

Monodisperse spherical core-shell silica nanoparticles with solid core and mesoporous shell were synthesized by adopting silica particles as core host components and surfactant molecules as structure-directing agents for the mesoporous shell. Here, two different types of surfactant molecules, octadecyltrimethoxysilane (C18-TMS) and cetyltrimethylammonium bromide (CTAB) were utilized as porogens for the formation of mesoporous shell over the spherical silica particles. Interestingly, while the C18-TMS generated uniform core-shell silica nanoparticles with disordered mesoporous shell, the CTAB produced core-shell silica nanoparticles with ordered mesoporous shell and the CTAB/PVP generated uniform core-shell silica nanoparticles with onion-like mesoporous shell. Monodisperse spherical core-shell (SCMS) silica particles with various mesoporous shell were synthesized by adopting silica particles as core host components, surfactant molecules as structure-directing agents for the mesoporous shell and polymer molecules as additives for shell structure. Here, we reported three different types of mesoporous shell structure. The synthesis of uniform spherical silica particles with disordered, ordered and paralleled mesoporous shell was demonstrated by employing different structure-directing molecules for the formation of mesoporous shell.

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## Transparent suspension of inorganic nanophosphor for displays

조영식, 김명진, 허영덕

단국대 화학과

Transparent suspension of inorganic nanophosphor ( $\text{YVO}_4\text{:Eu}$ ,  $\text{CaMoO}_4\text{:Tb}^{3+}, \text{Na}^+$ , and  $\text{BaMoO}_4\text{:Eu}^{3+}, \text{Na}^+$ ) were prepared using a surfactant-assisted hydrothermal reaction. Monodispersed nanoparticles of 10 ~ 15 nm in diameter were obtained by capping of oleic acid and oleylamine surfactants. A highly transparent suspension was obtained by dispersing the nanophosphor in toluene, which was stable after being left to stand for several weeks. This suspension was found to be suitable for transparent red ( $\text{YVO}_4\text{:Eu}$ ,  $\text{BaMoO}_4\text{:Eu}^{3+}, \text{Na}^+$ ) or green ( $\text{CaMoO}_4\text{:Tb}^{3+}, \text{Na}^+$ ) emitting phosphors by excited UV light. A simple and efficient method for fabrication of the flexible and transparent display devices was also confirmed by preparing a nanophosphor coated layer on overhead film.

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## Morphology-controlled synthesis of $\text{Cu}_2\text{O}$ and their physical properties

이용정, \*허영덕

단국대 물리화학 \*단국대 화학과

$\text{Cu}_2\text{O}$  microcrystals with specific morphology were synthesized by the reduction of a copper–ligand complex solution with glucose under microwave irradiation using various amines as ligands. Cube, octahedron, truncated octahedron, and hexapods of  $\text{Cu}_2\text{O}$  were obtained by changing the microwave irradiation time and the concentration of amine. SEM and XRD confirmed that the surfaces of the cubic and octahedral of  $\text{Cu}_2\text{O}$  microcrystals had  $\{100\}$  and  $\{111\}$  lattice planes. The morphology dependence of antibacterial activities and photocatalytic properties of the  $\text{Cu}_2\text{O}$  microcrystals were examined.



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## Morphology dependent photocatalytic activity of $\text{ZnWO}_4$

김명진, 허영덕

단국대 화학과

$\text{ZnWO}_4$  with various morphologies were synthesized by a ligand-assisted hydrothermal reaction. The choice of ligand was important for the formation of  $\text{ZnWO}_4$  rods. As increasing the strength of ligands, the aspect ratio of the  $\text{ZnWO}_4$  rods increases. XRD and HRTEM confirmed that the  $\text{ZnWO}_4$  rods grow along the [1 0 0] direction. The photocatalytic activities towards degradation of Rhodamine 6G under UV irradiation have been investigated. The photocatalytic activity was found to depend on the aspect ratio of  $\text{ZnWO}_4$  rods.

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## **Application of layered rare-earth hydroxides for removal of phosphate from aqueous solution.**

이수연, 변송호

경희대 화학과

Adsorption of phosphate by layered rare-earth hydroxides (LRHs) such as  $\text{Gd}_2(\text{OH})_5\text{Cl} \cdot n\text{H}_2\text{O}$  and  $\text{Y}_2(\text{OH})_5\text{Cl} \cdot n\text{H}_2\text{O}$  was investigated. LRHs were found to have high anion exchange capacity that enhances their capability to remove anionic contaminants from aqueous system. More particularly, we have found that P at a concentration below 5 ppm can be very efficiently and quickly removed through intercalation into the interlayer of LRHs, with less than 0.5 ppm of P left in solution. Therefore, LRHs are potential cost-effective adsorbent for trace phosphate. Furthermore, the analyses of the uptakes in mixed aqueous solution containing  $\text{NO}_3^-$ ,  $\text{CO}_3^{2-}$ , and  $\text{SO}_4^{2-}$  showed that the adsorbent had a markedly high selectivity for the adsorption of phosphate ions.

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## **Fabrication of Monodisperse Carbon Capsules with Hollow Macroporous Core/Mesoporous Shell: Morphological control of mesopores**

김윤경, \*김정호, \*김민식, \*\*chaudhari kiran, Nitin Chaudhari, 송민영, \*\*\*양대수, 최은지,  
\*유종성

고려대 소재화학과 \*고려대 신소재화학과 \*\*고려대 소재화학 \*\*\*고려대 신소재화학

Mesoporous materials have attracted much attention because of their emerging applications in catalysis, adsorption, sensors, and biotechnologies. The successful control over the composition and pore structure of mesoporous materials is the key factor for their functionalities. Mesoporous materials with very large pores are in urgent demand for applications in the encapsulation and separation of proteins where biomolecules with large molecular weights are involved. Moreover, our recent results revealed that their ordered large mesopores are promising for developing a highly efficient device for proteolysis reactions. In this paper, for the monodispersed solid core/ordered mesoporous shell (SCOMS) silica and pore size control of the mesoporous silica shell by using of different surfactants. Here, three different types of surfactant molecules, cetyltrimethylammonium bromide(C16-TMABr) and Brij 56/C16-TMABr and 1,3,5-trimethylbenzene(TMB) /decane/C16-TMABr were utilized as porogens for the formation of mesoporous shell over the spherical silica particles. In addition to hollow core/ordered mesoporous shell (HCOMS) carbon replica. Transmission electron microscopy (TEM), Scanning electronic microscopy (SEM) and nitrogen adsorption-desorption analysis are applied to characterize the synthesized HCOMS carbon.

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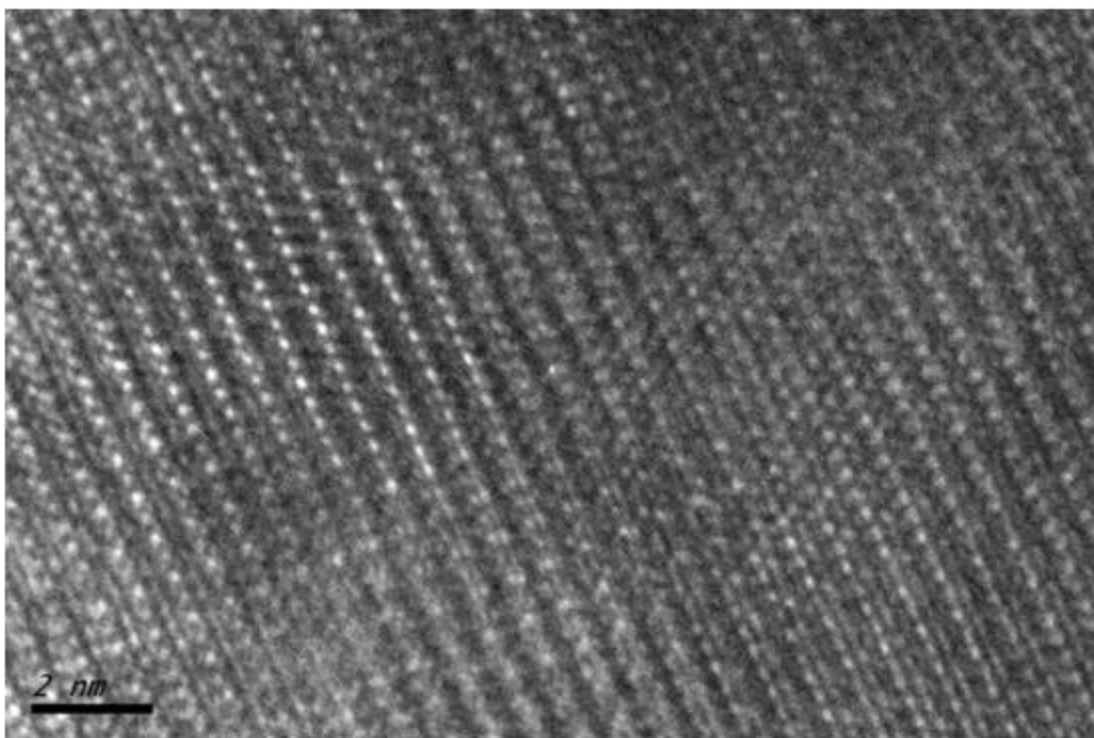
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## Characterization and microstructures of Bi<sub>2</sub>Te<sub>3</sub> prepared by insertion of Ni nanoparticles

김희진, 한미경, \*김성진

이화여대 화학나노과학부 \*이화여대 화학과

The thermoelectric device ability is measured by figure of merit (ZT). ZT is given by  $ZT = S^2 \sigma T / \kappa$  (where  $\sigma$  is the electrical conductivity,  $S$  the thermo power, and  $\kappa$  is the thermal conductivity) For several decades, the ZT of the thermoelectric materials have been less than 1. Current research results often are reported  $ZT > 2$  due to quantum confinement effect. We studied thermoelectric properties of Bi<sub>2</sub>Te<sub>3</sub> prepared by insertion of Ni nanoparticles. The thermal conductivity and the electrical conductivity decrease with increasing Ni nanoparticles contents. The phonons and electrons would be scattered by Ni nanoparticles depending on their contents. The contents of Ni nanoparticles are critical factor for achieving an increase in ZT compare to Bi<sub>2</sub>Te<sub>3</sub> bulk. An increase in ZT could be achieved for optimal contents of Ni nanoparticles. Seebeck coefficient and electrical conductivity have been measured by ZEM-3(Ulvac) and the thermoelectric figure merit calculated. The microstructure and morphologies of Bi<sub>2</sub>Te<sub>3</sub> insertion of the Ni nanoparticles were investigated by Powder X-ray diffraction(Rigaku D/MAX X-ray) and HR-TEM(High resolution Transmission electron microscopy, JEOL 2100F)



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## Synthesis of Bi<sub>2</sub>Te<sub>3</sub> nanoparticles : shape control and characterization

김솔, \*성은규, \*\*오은영, \*\*\*한미경, 김성진

이화여대 화학과 \*이화여대 화학나노과학과 \*\*이화여대 화학, 나노과학과 \*\*\*이화여대 화학나노과학부

Bismuth telluride (Bi<sub>2</sub>Te<sub>3</sub>) is one of the promising thermoelectric materials at room temperature. Recent improvements in thermoelectric efficiency are dominated by efforts to reduce the lattice thermal conductivity through introducing nanostructured phase. The effect of nanostructures on the phonon scattering is determined by a set of physical parameters such as its size, shape and composition. Therefore, a good control over these parameters is essential in achieving further improvements in thermoelectric efficiencies. We obtained monodisperse Bi<sub>2</sub>Te<sub>3</sub> nanoparticles with different morphology by controlling the relative ratio of capping agent and Bi-Te precursor, reaction temperature, time and pressure. The size of the particles is around 10nm when their shape is sphere and 50nm in case of cubic. The synthesized various nanostructures are investigated by using HR-TEM, SEM and XRD analysis. Bi<sub>2</sub>Te<sub>3</sub> nanostructures with different shape are expected to have potential applications in a variety of areas including high efficiency thermoelectric devices.

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## Graphene as an effective catalytic layer toward the nanowire growth

박지은, \*김경, \*김여진, \*이유민, \*\*이재연, 김명화, \*\*\*김성진

이화여대 화학 나노과학과 \*이화여대 화학나노과학과 \*\*이화여대 화학·나노과학과 \*\*\*이화여대 화학과

We report a new strategy to use graphene layers as a catalytic substrate for effective growth of RuO<sub>2</sub> nanowires. Using this method, the high density of single crystalline RuO<sub>2</sub> nanowires were exclusively obtained on the graphene layers transferred onto a SiO<sub>2</sub>/Si(100) substrate with the lateral dimension of 20 – 150 nm and the length of more than 10 μm long. We tentatively suggest that this enhanced nanowire growth can be attributed to the formation of a significant number defects in the basal plane of graphene under high temperature and O<sub>2</sub> environment based on Raman measurements. Indeed, the preferential nucleation process of the precursor gas molecules during chemical vapor deposition (CVD) growth can be effectively occurred from these highly activated defects of graphene layers. This rational engineering of graphene layers to generate numerous defects may thus provide a promising method for producing highly-dense 1dimensional nanomaterials.

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## Effects of Surface Roughness on the Thermoelectric Properties of $\text{Bi}_2\text{Te}_3$ Nanowire

김하영, \*김소영, 김성진

이화여대 화학과 \*이화여대 화학나노과학과

We synthesized bismuth telluride ( $\text{Bi}_2\text{Te}_3$ ) nanowires with different surface roughness by pulsed-potential deposition using  $\text{Bi}(\text{NO}_3)_3 \cdot 5\text{H}_2\text{O}$  and  $\text{TeO}_2$  in 1.0 M  $\text{HNO}_3$  in porous anodic alumina template at room temperature. Obtained nanowires show smooth or rough surface with the diameter of about 150 nm. The pulse potentials for nanowires synthesis were selected more negative potential than the reduction potential observed from cyclic voltammograms (CVs), the delay potential was used in no current region between reduction and oxidation potentials of the compound. We observed that the growth rate is critical factor to obtain dense, highly oriented single-crystalline nanowires. Pulsed-potential influence atomic ratio of compound, and pulsed-time can affect the crystallinity of nanowires. We can control the surface roughness of the nanowires by changing stirring rate of the electrolyte. The microstructures and morphologies of nanowires were investigated by powder X-ray diffraction, FE-SEM, and HR-TEM. Electrical conductivity, thermal conductivity, and thermal contact resistance of the nanowires were measured for both morphology samples. Regardless of the surface roughness, nanowires have the similar electrical conductivity values, whereas nanowire with rough surface show more reduced thermal conductivity at room temperature compared to smooth one.



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발표종류: 포스터, 발표일시: 목 10:30~12:30

## Transfer of graphene films using direct deposition polymer

김창현, 최진웅, 조용재, 박정희

고려대 소재화학과

We report the new transfer method of graphene layers on metal substrate. We demonstrate the transfer and exfoliation of graphene layers on metal substrate by direct deposition polymer. First of all we prepared multilayer graphene grown on Co foils by chemical vapor deposition and PDMS substrate cured in vacuum oven for 1hour. After transfer, we measured Raman spectra and absorption spectra to verified number of remaind graphene layer on metal, polymer substrate. As a result of experiment, we discovered to control from single graphene layer to ten layers through transfer. This simple technique can be used to controllably transfer graphene layer for property studies, for the fabrication of devices.

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## Visualized Graphene Domains by Aligned Nematic Liquid Crystals

김대우, \*정현수, \*정희태

KAIST 생명화학공학과 \*KAIST 생명화학공학과

Direct visualization of large-area graphene domains is one of the key issues in graphene research, because their electronic, magnetic, chemical and mechanical properties are dominated by their domain size and direction of hexagonally packed carbon matrix. All previous methods used to visualize the domain and boundary of graphene, which include atomic force microscopy, scanning electron microscopy, transmission electron microscopy and raman spectroscopy, are only effective for small area up to several micrometer. This is unable to determine the domain size of the large-area graphene. Here, we demonstrate a very simple method to macroscopically visualize the graphene domains and their boundaries by using nematic liquid crystals on the surface of graphene. Epitaxially aligned nematic liquid crystals on graphene surface are observed using polarized optical microscopy, and obtained textures from liquid crystals are well matched with the domain of graphene. Using this approach, we investigated the effect of domain size and boundary on the quality of graphene in terms of conductance. This method will open a new window for studies on the control of domain, boundary and structure and properties of graphene.

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발표종류: 포스터, 발표일시: 목 10:30~12:30

## Highly Oriented Growth of Single-Crystalline Cobalt Nanowires by Chemical Vapor Transport Method

김시인, 김현주, 김봉수

KAIST 화학과

Highly oriented, single-crystal Co nanowire(NW) arrays have been synthesized on a m-plane sapphire substrate using a single-step chemical vapor transport method in absence of any foreign catalyst. Electron and X-ray diffraction confirm the single crystallinity of the Co NWs with fcc crystal structure. Furthermore, Co NW is converted to  $\text{Co}_3\text{O}_4$  nanotube (NT) by high temperature thermal annealing in diluted  $\text{O}_2$  condition. Transmission electron microscopy(TEM) studies show distinct change of the nanostructure morphology and composition. A transformation mechanism involving overlapping oxidation and thermal diffusion is presented. The ferromagnetic vertical Co NWs can be employed as an important building block in the development of high density storage media. In addition, since  $\text{Co}_3\text{O}_4$  is an important magnetic p-type semiconductor with a normal spinel structure, it has many commercial or potential applications as heterogeneous catalysts, anode materials in Li-ion rechargeable batteries, solar energy absorbers and soon.

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발표종류: 포스터, 발표일시: 목 10:30~12:30

## Synthesis and characterization of binary to quaternary Nb-based compound nanowires

김현주, 김봉수

KAIST 화학과

We report the synthesis of binary to quaternary niobium-based germanide silicide nanowires (NWs). To achieve multi-component NWs from binary NWs, we controlled the NWs growth temperature and employed the metal foils as a substrate and a precursor in this experiment. We observed that the ternary and quaternary NWs have ordered phase by Cs-corrected scanning transmission electron microscope (STEM) measurement. In addition, quaternary NWs ensemble shows superconducting properties by superconducting quantum interference device (SQUID) measurement. To reconfirm this result, we have been measuring the electrical and magnetic transport of individual quaternary compound NWs.

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발표분야: 재료화학

발표종류: 포스터, 발표일시: 목 10:30~12:30

## Synthesis of Iron-based chalcogenide nanostructures as a candidate material for superconductor

김현주, 김봉수

KAIST 화학과

We report the synthesis of single crystal  $\text{Fe}_9\text{Te}_8$  nanowires and nanoplates in a chemical vapor deposition (CVD) method. In addition, we observed that the  $\text{Fe}_9\text{Te}_8$  nanostructures have layered structure by Cs-corrected scanning transmission electron microscope (STEM) measurement. We expect to superconductivity in  $\text{Fe}_9\text{Te}_8$  nanostructures, so we have been measuring the magnetic transport of individual  $\text{Fe}_9\text{Te}_8$  nanostructures to confirm the superconductivity.

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## **The development of a novel laser desorption/ionization platform composed of graphene oxide and nanostructured gold for efficient small molecules**

김영관, 민달희

KAIST 화학과

The oxidized form of graphene, graphene oxide (GO), is an important and promising material providing high water solubility and interesting optical properties such as strong UV-absorption, fluorescence and surface enhanced Raman scattering. Those optical properties render graphene oxide actively used for various applications such as biosensor, non-linear optics, surface enhanced Raman scattering and matrix free laser desorption/ionization mass spectrometry (LDI-MS). In this work, we develop a novel nanohybrid platform composed of GO and nanostructured gold for efficient LDI-MS analysis of small molecules because GO and gold nanomaterials can be employed as an efficient matrix and form strongly interactive structure for synergy effect. The nanohybrid platform was fabricated by surface immobilization of GO sheets on a glass substrate and subsequent surface growth of gold nanostructure via seed-mediated growth approach. The fabricated nanohybrid platform was systematically characterized by SEM, AFM, UV-vis and Raman spectroscopy and LDI-MS to reveal interaction mode at interfacing points and performance as a LDI-MS platform. The nanohybrid platform showed excellent performance when it was used to analyze small molecules by LDI-MS with good ion tolerance, even spatial signal distribution and structural durability. We believe that this nanohybrid platform will be one of the efficient tools for LDI-MS analysis of small molecules because of its excellent performance, cost-effectiveness and simple fabrication processes.

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## Optical and Catalytic Properties of Encapsulated Silicon Oxynitride Nanoparticles in a Mesoporous Silica Microsphere

유정보, 임병욱, 이강혁, 유효진, 최종명, \*채원식, \*\*한옥희, 허남희

서강대 화학과 \*한국기초과학지원연구원 강릉센터 \*\*한국기초과학지원연구원 대구센터

Encapsulated silicon oxynitride nanoparticles (NPs),  $\text{SiO}_{2-x}\text{N}_x@ \text{SiO}_2$ , were prepared by annealing the mesoporous core/shell silica microsphere under the  $\text{NH}_3/\text{Ar}$  atmosphere at  $700^\circ\text{C}$  for 12 h. Photoluminescence, time-resolved fluorescence, transmission electron microscope,  $^{29}\text{Si}$  MAS solid state NMR, XPS, and nitrogen absorption isotherms were employed to characterize the  $\text{SiO}_{2-x}\text{N}_x@ \text{SiO}_2$  NPs. The spectroscopic data reveal that the oxygen in the shell might be partially replaced by nitrogen or  $\text{NH}_x$  moieties. The partial substitution of oxygen in silica surface by nitrogen species leads to the formation of silicon oxynitride NPs within the mesoporous shell. The encapsulated oxynitride NPs show an excellent catalytic activity for the Knoevenagel condensation reaction between benzaldehyde and malonitrile. Another notable feature is that they exhibit distinctive broad luminescence signals in the range of 300 to 550 nm.

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발표종류: 포스터, 발표일시: 목 10:30~12:30

## His-tagged Enzyme Conjugated Magnetic Mesoporous Silica For High Efficient Biodegradation of Catechol

이지호, 박상언, \*장정호

인하대 화학과 \*요업기술원 바이오IT융합센터

In this study, we will present a novel method for mesoporous silicas which are functionalized with Fe and Ni ion to support His-tagged proteins. Mesoporous silicas were combined with iron(II) chloride tetrahydrate for initiating magnetizing process, followed by reduction in H<sub>2</sub> media. The nickel(II) chloride hexahydrate was introduced into pore and surface of magnetic mesoporous silicas(MMS) by wet impregnation process. The resulting materials were reduced in a flowing of H<sub>2</sub> at 500 °C for 2h, thereby producing Ni particles on the surface of the MMS. The Ni particles were oxidized by exposing them to the air under ambient conditions for two days. The Ni-MMS was characterized by various state-of-the-art techniques, such as SAXS, WAXS, FE-SEM, TEM, FT-IR, SQUID and nitrogen sorption. Ni-MMS showed high adsorption level of His-tagged protein from E.coli lysate. In addition, the purified His6-CatA was observed high enzyme activity. It suggests that Ni-MMS system provides contribution for maintain stable protein structure as well as simplified protein purification process.



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## **Influence of Polystyrene Grafted Multi-walled Carbon Nanotubes on Viscoelastic Properties of Polypropylene Based Nanocomposites**

심영선, 박수진

인하대 화학과

In this work, a free-radical grafting method was applied for the modification of multi-walled carbon nanotubes (MWNTs) to improve their dispersion in polypropylene matrix. PS-MWNTs nanostructure was synthesized by the in situ free-radical polymerization of styrene monomer on the surface of MWNTs. PS-MWNTs/PP nanocomposites were prepared by melt mixing. The effect of polystyrene grafted multi-walled carbon nanotubes (PS-MWNTs) content on the polypropylene (PP) based nanocomposites was investigated. And surface characteristics of PS-MWNTs were examined by infrared spectroscopy, Raman spectroscopy (FT-Raman), thermogravimetric analysis (TGA) and transmission electron microscopy (TEM). The rheological properties of PS-MWNTs/PP composites were confirmed by rheometer. As a result, grafted PS was affected to show the increases rheological properties. It is considered because of in situ free-radical polymerization, MWNTs agglomerates turn into a networked micro-structure, which in turn builds up a strong interfacial interaction with the polymeric matrix during the mixing procedure.

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## Effect of Polypropylene Grafted Multi-walled Carbon Nanotubes on Rheological Properties of Polypropylene Nanocomposites

심영선, 박수진

인하대 화학과

In this study, the grafting technique of organic species to improve the dispersion of multi-walled carbon nanotubes (MWNTs) in polypropylene (PP) matrix. PP grafted MWNTs composites (PP-g-MWNTs) were prepared by reaction with melt mixing between PP grafted maleic anhydride (PP-g-MA) and acid treated MWNTs. The effect of PP-g-MWNTs content on rheological properties of PP-g-MWNTs/PP nanocomposites was investigated. As a result, the extent of enhancement in rheological properties of PP-g-MWNTs/PP above 5 wt% of PP-g-MWNTs decreased due to an apparently increased tendency of clustering of carbon nanotubes. Thus, it is considered that attached PP on the surface of MWNTs influence to increase compatibility between MWNTs and PP matrix.

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발표종류: 포스터, 발표일시: 목 10:30~12:30

## Zinc Stabilized Cubic Copper Ferrites and Their Catalytic Activity

김미현, 이규형, 강승희, 강동현, 허남희

서강대 화학과

Spinel ferrites,  $AFe_2O_4$ , have widely been studied since they possess interesting magnetic properties depending on the A ion. Most of spinel ferrites adopt cubic structure. In the case of copper ferrite ( $CuFe_2O_4$ ), however, it typically crystallizes as a tetragonal structure due mainly to the Jahn-Teller distortion induced by the  $Cu^{2+}$  ion. In the present study zinc is employed to the Cu site, which results in the stabilization of the cubic structure. We isolated cubic  $(Cu_{1-x}Zn_x)Fe_2O_4$  nanoparticles (NPs) with the average particle size of 6 nm by co-precipitation method, which were characterized by transmission electron microscopy, powder X-ray diffraction, and SQUID magnetometer. The cubic copper ferrite NPs also show high catalytic activity in N-formylation of amine.

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발표종류: 포스터, 발표일시: 목 10:30~12:30

## Epitaxially-driven Stereoaligned Growth of Pt Nanowires from Oriented Seed Crystals

유영동, 강태준, 김봉수

KAIST 화학과

Epitaxial Pt nanowire (NW) arrays are synthesized for the first time via a chemical vapor transport method using a metal halide as a precursor. Here we report that the epitaxial growth direction of NWs can be steered by seed crystal morphology. Octahedral seeds grow into inclined NWs possessing six growth directions, while half-octahedral seeds grow into vertical and horizontal NWs. Interfacial energies between the seed material and the substrate are critical in determining the morphology of seed crystals. We also demonstrate that non-SERS-active Pt NWs can show strong surface enhanced Raman scattering (SERS) spectra by placing them on Ag films. The active SERS observation would help to elucidate Pt-catalyzed chemical reactions.

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발표종류: 포스터, 발표일시: 목 10:30~12:30

## **CO<sub>2</sub> Adsorption Properties of As-made Mesostructured Silicas Prepared from Primary Amine Porogens**

김미지, \*박인

연세대 화공생명공학과 \*한국생산기술연구원 패키징기술지원센터

As-made mesoporous silicas assembled in the presence of primary amine porogens were synthesized to be used as CO<sub>2</sub> adsorbents. Unlike conventional PEI(Polyethylenimine)-impregnated mesoporous silicas, the primary amine porogens in the pore of the as-made mesoporous silicas can adsorb CO<sub>2</sub> molecules without need for calcination and PEI impregnation. HMS (wormhole) and MSU-SA (lamella) were prepared from a monoamine surfactant (dodecylamine). MSU-J (wormhole), MSU-V and MSU-G (lamellar vesicles) synthesized from diamine surfactants were also used as CO<sub>2</sub> adsorbents to increase amine content and adsorption capacity. PEI(polyethylenimine)-impregnated as-made mesoporous silicas were also examined for CO<sub>2</sub> adsorption. Macropore in the center of the vesicular framework structure (MSU-V and MSU-G) provides sufficient space for PEI loading.

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발표종류: 포스터, 발표일시: 목 10:30~12:30

## **Doxorubicin Delivery Efficiency of Dextran-coated Gold Nanoparticles against Size Variables**

장홍제, 유수윤, 민달희

KAIST 화학과

Gold nanoparticles (AuNPs) have been actively harnessed in many bio-applications for developing sensors, diagnostics, and drug delivery vehicles. In previous research, we developed facile synthetic strategy to prepare gold nanoparticles for biological applications that require biocompatibility and excellent colloidal stability against heat, high salt concentrations and extreme pH conditions by using biocompatible polymer dextran as a reducing agent and surface coating. Here, we report successful control over the size of dextran coated gold nanoparticles (Dex-AuNPs) by varying the concentrations of Au(III) solution during the particle synthesis. Cross-linking and amination of dex-AuNPs significantly improved the colloidal stability and rendered the nanoparticles more appropriately to bioconjugations. Fluorescence dye Cy 5.5 and anticancer drug doxorubicin were sequentially conjugated to various sized aminated dex-AuNPs (N-cl-dex-AuNPs). The dox-Cy5.5-n-cl-dex-AuNPs complex was readily internalized into HeLa cells and induced apoptosis. MTT cell viability assay revealed that the delivery efficiency was improved over 5,000 times compared with free doxorubicin. The result suggests that our dextran coated AuNPs have high potential as an effective drug carrier for biocompatible drug delivery system.

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## Enzyme-mimic magnetic catalysts for high throughput hydrolysis of p-nitrophenyl esters by biomimetic catalysts

이선영, 박상언, \*장정호

인하대 화학과 \*요업기술원 바이오IT융합센터

The work reports the development of the high throughput hydrolysis of p-nitrophenyl esters with enzyme-mimic catalysts which are originated from silica coated magnetic nanoparticles. Magnetic nanoparticles were prepared by coprecipitation of  $\text{Fe}^{2+}$  and  $\text{Fe}^{3+}$  and then tetraethyl orthosilicate was directly coated by sol-gel process. Functional groups such as amine, carboxyl, imidazol groups were grafted on the magnetic nanoparticles surface mimicking a triads of Ser 195, His 57, Asp 102 of chymotrypsin. These groups were required for enhanced catalytic activity toward the hydrolysis of ester. To compare catalytic activity with biocatalysts, hydrolysis of p-nitrophenyl esters were observed by UV-visible spectrophotometer. The result showed that the hydrolysing property enzyme-mimic magnetic catalysts were more enhanced than chymotrypsin. It suggests that enzyme-mimic magnetic catalysts might be used biocatalysts or biosensors application.

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## Hollow Core Mesoporous Shell Carbon as a support for Pt-Fe alloys cathode catalyst in Proton Exchange Membrane Fuel Cell

송민영, \*김정호, \*\*양대수, 김윤경, \*김민식, 박진솔, \*권선영, Nitin Chaudhari,  
\*\*\*chaudhari kiran, \*유종성

고려대 소재화학과 \*고려대 신소재화학과 \*\*고려대 신소재화학 \*\*\*고려대 소재화학

Hierarchical nanostructured spherical carbon with hollow macroporous core in combination with mesoporous shell has been explored to support Pt-Fe alloys cathode catalyst with high metal loading in proton exchange membrane fuel cell (PEMFC). The HCMS carbon consisting of discrete spherical particles possesses unique structural characteristics including large specific surface area and mesoporous volume and well-developed interconnected void structure, which are highly desired for a cathode catalyst support in low temperature fuel cells. In this strategy, HCMS Carbon was further used to support high loading of Pt-Fe alloy nanoparticles (NPs) through a urea-assisted homogeneous deposition (HD) strategy by using ethylene glycol (EG) as the precursor of a reducing agent. The HCMSC-supported Pt-Fe(60 wt%) cathode catalysts has demonstrated markedly enhanced catalytic activity toward oxygen reduction and greatly improved PEMFC polarization performance compared with carbon black Vulcan XC-72(VC)-supported ones.



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## Colloid-imprinted carbon with superb nanostructure as an efficient anode materials for lithium ion batteries

양대수, \*송민영, \*\*김정호, \*김윤경, \*최혁수, \*\*유종성

고려대 신소재화학 \*고려대 소재화학과 \*\*고려대 신소재화학과

Novel colloid-imprinted carbon material CIC-22 with tailored mesopore size of ca. 22 nm was explored for anode materials for lithium ion batteries. The CIC-22 possesses unique structural characteristics including nonmicropores, large specific surface area and pore volume, well-developed interconnected mesoporosity, and high electrical conductivity as well. This CIC-22 displays superior Li-battery performance with large reversible capacity, excellent cyclic performance, and good rate capability, and graphene for energy storage applications in high-performance lithium-ion batteries.

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## **Fe<sub>3</sub>O<sub>4</sub> Magnetic Nanoparticles and Oxidases Inside Nanoporous Silica as a Colorimetric Sensor**

심종민

포항공과대 화학공학과

We develop one-pot multi catalyst system, so called "nano-reactor", entrapping Fe<sub>3</sub>O<sub>4</sub> magnetic nanoparticles (MNPs) and oxidases in nanoporous silica with high loading simultaneously above 40 wt% MNPs and 20 wt% enzyme. The nano-reactor developed in the present work provided highly loaded MNP system and any highly loaded enzymes with superior activity, stability, and reusability, thereby making further applications as versatile sensors for detecting DNA, protein, and cell highly promising

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발표종류: 포스터, 발표일시: 목 10:30~12:30

## Surface modification of Tungsten nanopowder and its wettability in HDPE/EPM matrix

염영랑, \*김재우, \*\*전지현, \*배연주

한국원자력연구소 원자력재료개발부 \*한국원자력연구원 원자력재료개발부 \*\*한국원자력연구소 원자력 재료개발부

To improve dispersion strength and wettability of the nanoparticles in polymer, the hydrophobic surface modification is demanded. Low density polyethylene (LDPE) and Octadecyl-trichloro-silane (OTS) were chosen as a surface treatment agent. LDPE was dissolved in the organic solvent of cyclohexane. After LDPE powder was completely dissolved in cyclohexane, W powder was added. OTS and W particles were dissolved and dispersed in toluene solvent. The ultrasonic treatment for the OTS dissolved solvent was carried out at room temperature. The surface modified particles were reinforced in HDPE/EPM polymer by using twin screw extruder with co-rotating blades. The mechanical properties such as tensile strengths and elongations of both LDPE and OTS coated W particles dispersed HDPE/EPM sheets were measured and estimated. LDPE coated W particles dispersed polymer sheet showed more strong mechanical properties than OTS treated particles dispersed one, due to relatively enhanced adhesion between filler and matrix. It results in surface modified material of LDPE is same material of polymer matrix.

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발표코드: I-MAT.P-274

발표분야: 재료화학

발표종류: 포스터, 발표일시: 목 10:30~12:30

## Nanoballs within nanoballs

윤경원, 백강균, 김기문

포항공과대 지능초분자 연구단, WCU 첨단재료과학부, 화학과

We recently reported a one-pot, template-free synthesis of polymer nanocapsules.<sup>1</sup> As an extension of this work, we now report the one pot, direct synthesis of nanoballs within nanoballs, which are composed of semiconductor nanoparticles encapsulated in a polymer nanocapsule. When the nanocapsule formation reaction was carried out in the presence of the nanoparticles, they are trapped inside the nanocapsules. The successful construction of nanoballs within nanoballs has been confirmed by transmission electron microscopy and other techniques. Such nanoballs within nanoballs may find useful applications in many areas including optical devices, catalyst, solar cell, and medical imaging. Details of the synthesis and characterization of the nanoballs within nanoballs will be presented. 1. (a) Kim, D.; et al. *Angew. Chem., Int. Ed.* 2007, 46, 3471–3474. (b) Kim, D.; Kim, E.; Lee, J.; Hong, S.; Sung, S.; Lim, N.; Park, C. G.; Kim K. *J. Am. Chem. Soc.* 2010, 132, 9908–9919.

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발표종류: 포스터, 발표일시: 목 10:30~12:30

## Facile, template-free synthesis of nanorings through irreversible covalent bond formation

이지영, 홍순상, 백강균, 윤경원, 김기문

포항공과대 지능초분자연구단, WCU 첨단재료과학부, 화학과

We have recently developed a new, direct synthetic method of polymer nanocapsules through irreversible covalent bond formation between a rigid disk-shaped molecule with isotropic multiple polymerizable groups and dithiols without using any template or pre-organized structure.<sup>1</sup> A proposed mechanism of the nanocapsule formation involves 2D oligomeric patches initially formed as a result of the edge-to-edge connection of dimers and trimers of the monomer, turning into a hollow sphere.<sup>2</sup> While investigating various factors affecting the nanocapsule formation we found other interesting nanostructures including nanorings. Here we present the direct synthesis of nanorings by thiol-ene “Click” reaction between 2,3,6,7-tetrakis(allyloxy) anthracene-9,10-dione, a rigid, rectangular-shaped molecule with polymerizable allyloxy groups and dithiols without any templates. The resulting nanorings have been characterized by various techniques including AFM, SEM and TEM. The details of the synthesis and characterization of the nanorings will be presented. (1) Kim, D.; et al. *Angew. Chem. Int. Ed.* 2007, 46, 3471–3474. (2) Kim, D.; Kim, E.; Lee, J.; Hong, S.; Sung, W.; Lim, N.; Park, C. G.; Kim, K. *J. Am. Chem. Soc.* 2010, 132, 9908-9919.

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## Synthesis and Characterization of Poly(*N*-isopropylacrylamide)- Magnetic liposomes

김원희, 박상언, \*장정호

인하대 화학과 \*요업기술원 바이오IT융합센터

This work describes a synthesis of temperature-responsive poly(*N*-isopropylacrylamide)-magnetic liposomes. We utilized the coacervation method to form liposomes. Liposomes were synthesized by using lecithin and ferric ions, and then silicified the liposomes. The silicified liposomes were magnetized by streaming hydrogen gas at 800°C. Temperature-responsive poly(*N*-isopropylacrylamide) and magnetic liposomes were conjugated by UV polymerization method. As a result, particle size of magnetic liposomes was in the range of 200~600nm and particle size of poly(*N*-isopropylacrylamide)-magnetic liposomes was 400~800nm. The characterization of these materials was investigated by TEM, DLS, FR-IR, SEM-EDX and XRD analysis. These materials can be used for biomedical application such as drug delivery system.

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## Structure-Directing Surfactant-Driven Crystallization of Hierarchically Nanoporous Zeolites

나경수, 유 룡

KAIST 화학과

Synthesis of mesoporous ( $2\text{ nm} < \text{pore diameter} < 50\text{ nm}$ ) molecular sieves built with crystalline microporous ( $0.3 < \text{pore diameter} < 1.5\text{ nm}$ ) zeolitic framework has been a long-cherished task in nanoporous materials science and related industrial technology. Such hierarchically nanoporous zeolites have been demonstrated to resolve the limitation of zeolite use and further widen the application regime of microporous zeolite to the mesoporous-length scales. Herein, a series of hierarchically nanoporous zeolites have been synthesized by using a structure-directing surfactant, where a surfactant functionalized with a specific zeolite structure-directing group was used as a hierarchical nanopore-generating agent. During the crystallization process, the zeolite structure-directing group directs a specific microporous topology such as MFI, BEA and MTW, while the surfactant micellization constructs a various types of mesostructures such as hexagonal, lamellar and disordered phases. Notably, it is possible to systematically and also uniformly control the crystal thickness of microporous framework (i.e., mesopore wall) in the range of 1.7 to 5.1 nm in proportion to the length of zeolite structure-directing fraction in the surfactant. In addition, the mesopore diameter can be controlled over a wide range of mesopore regime (3.7 ~ 21 nm) by the addition of mesopore-swelling agent such as 1,3,5-trimethylbenzene. The resultant hierarchically nanoporous zeolites would exhibit many synergies of crystalline zeolitic framework and mesoporous architecture.

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발표분야: 재료화학

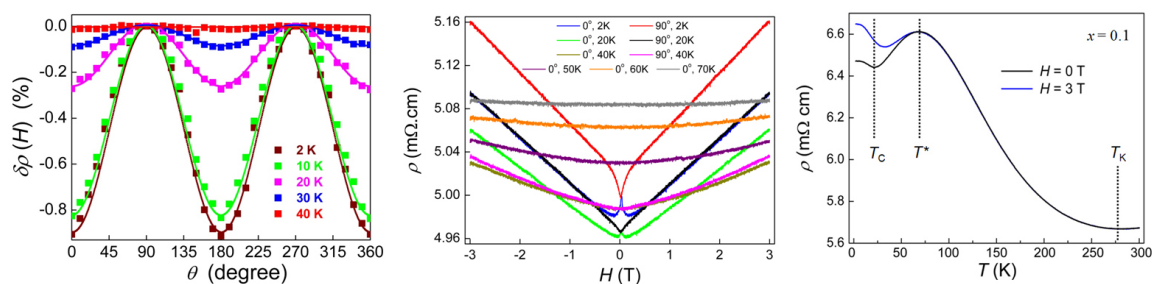
발표종류: 포스터, 발표일시: 목 10:30~12:30

## Negative Anisotropic Magnetoresistance and Kondo Effect in a Ferromagnetic Single-Crystalline Fe<sub>1-x</sub>CoxSi Nanowire

이성훈, 김봉수

KAIST 화학과

We report unconventional magneto-transport properties of an individual Fe<sub>1-x</sub>CoxSi nanowire. We study the angle between the directions of the magnetization and electrical current dependent resistivity below Curie temperature. Observed anisotropic magnetoresistance ratio indicates a negative value, which is consistent with that the conduction electrons in minority spin band of Fe<sub>1-x</sub>CoxSi nanowire transport dominantly. Positive magnetoresistance is shown in the overall temperatures range in contrast with typical ferromagnets. The shape-change of magnetoresistance curve is due to Zeeman splitting effect through the Curie temperature. With measuring temperature dependent resistivity, Kondo effect is observed in Fe<sub>1-x</sub>CoxSi nanowire. By synthesizing highly single-crystalline Fe<sub>1-x</sub>CoxSi nanowires we could observe suppression of Kondo effect in a lower dimensional structure and prominent intrinsic transport properties.





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발표종류: 포스터, 발표일시: 목 10:30~12:30

## **Synthesis and application of ordered mesoporous carbon for removal of chromium ions from aqueous solution**

김진희, \*김영훈, \*이영재, \*최진성, \*김순근, 김지만

성균관대 화학과 \*경기과학교

Herein, we fabricated ordered mesoporous carbon with high surface area has been used as a solid sorbent for the application to removal of chromium ion. First of all, the ordered mesoporous carbon was fabricated various carbon precursor which containing N or S atoms for adsorption of heavy metal ions by nano-replication technique. The N or S atoms are well known as adsorbable atoms for heavy metal removal by formation of metal-sulfide, metal-nitride or chelating species. And the adsorption experiment was carried out with various conditions of initial adsorbate concentration, adsorption time and adsorbent weight at 25°C, 200 rpm and 100mL solution. The ordered mesoporous carbons were characterized with X-ray diffraction, N<sub>2</sub> sorption, scanning electron microscopy, transmission electron microscopy, and adsorption ability was analyzed with UV-Vis spectrum and ICP.

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발표분야: 재료화학

발표종류: 포스터, 발표일시: 목 10:30~12:30

## **Fabrication of sulfonated mesoporous carbon for solid acid catalysis**

김진희, \*방준호, \*김영우, \*김순근, 김지만

성균관대 화학과 \*경기대학교

Herein, we fabricated ordered mesoporous silica as hard template by sol-gel synthesis and ordered mesoporous carbon by nano-replication technique with sulfur containing carbon precursor. In the silica removal sequence, surface modification with sulfonate group was appeared by hydrofluoric acid and we used the functionalized acid site for solid acid reaction. To compare, we synthesized reference ordered mesoporous carbon with sucrose as carbon precursor, and surface modified ordered mesoporous carbon by post treatment with sulfuric acid. However the ordered mesoporous carbon structure was damaged by post acid treatment sequence, so we fabricated Ia3d structure to maintenance the 3D pore network structure against collapsibility. The ordered mesoporous silica, carbon and post acid treated carbon were analyzed by X-ray diffraction, N<sub>2</sub> sorption, scanning electron microscopy, transmission electron microscopy, FT-IR and UV-Vis spectrum.

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발표분야: 재료화학

발표종류: 포스터, 발표일시: 목 10:30~12:30

## Greenish yellow phosphorescent OLEDs using iridium(III) complexes with phenylpyridine ligands containing dimethylsilyl group

강소희, 김철영, \*신민기, 김윤희, \*\*권순기

경상대 화학과 \*경상대 고분자공학전공 \*\*경상대 나노신소재공학부

Organic light-emitting diodes (OLEDs) have attracted great attention in the past decades because of their potential advantages in full-color displays. In particular, phosphorescent metal complexes have been considered to be promising materials because of their ability to achieve maximum internal quantum efficiency, nearly 100%, as well as high external quantum efficiency in OLEDs. In this research, we report the synthesis of iridium complex uniting trimethylsilyl group. Trimethylsilyl units is known for good solubility, thermal stability and steric bulk via higher volume. Therefore, the combination of ppy and bulky trimethylsilyl units would be expected to be the best way to achieve an efficient phosphorescent emitter. In this research, we report the synthesis of iridium complex uniting dimethylsilyl group. dimethylsilyl units is known for good solubility, thermal stability and steric bulk via higher volume. Therefore, the combination of ppy and bulky dimethylsilyl units would be expected to be the best way to achieve an efficient phosphorescent emitter.

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발표종류: 포스터, 발표일시: 목 10:30~12:30

## Synthesis and Properties of new Semiconductor oligomer containing Alkyl-naphthalene

박소민, \*신민기, \*고혜진, \*\*오대환, \*\*김윤희, \*\*\*권순기

경상대 고분자공학과 \*경상대 고분자공학전공 \*\*경상대 화학과 \*\*\*경상대 나노신소재공학부

Organic thin-film transistors (OTFTs) have undergone tremendous progress in the past decade. Compared with traditional silicon electronics, electronic devices based on OTFTs offer unique attractions, such as light weight, mechanical flexibility, and low-cost production. In the recent past, oligothiophenes and their alkyl-substituted derivatives have been among the most intensely investigated organic semiconductors and have even led to the demonstration of fast integrated circuits. Molecular ordering is believed to play a large role in the performance of devices based on these organic materials as active layer materials, especially for small molecular material, the amount of  $\pi$ -orbital overlap is expected to have a strong influence on field-effect mobility. In this study, we designed and synthesized a new oligomer containing alkyl-naphthalene (NBTDN) by well-known Suzuki coupling reaction. The obtained NBTDN was confirmed by <sup>1</sup>H NMR, FT-IR and Mass spectroscopic studies. The physical and optical properties of NBTDN were characterized using various studies such as cyclic- voltammetry (CV), UV-visible absorption and photoluminescence (PL) spectroscopic studies, and the results will be presented in detail. The high thermal stability of NBTDN was determined by thermogravimetric analysis (TGA) and differential scanning calorimeter (DSC) studies. The results showed that this new oligomer containing alkyl-naphthalene (NBTDN) can be a promising candidate for OTFT applications.

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발표종류: 포스터, 발표일시: 목 10:30~12:30

## Synthesis and Characterization of High Triplet Energy Host Material for OLED

오대환, 유승진, \*권순기, 김윤희

경상대 화학과 \*경상대 나노신소재공학부

Organic light-emitting device (OLEDs) have been the subject of intense academic and industrial research in recent years due to their potential advantages in high-efficiency, low-driving-voltage, full-color flat-panel display systems and next generation energy-saving light. In this research, we phosphine oxide and carbazole moiety for high triplet energy band gap( $E_T$ ), thermal-chemical stability, high efficiency and stability of a device. The material was characterized by  $^1\text{H-NMR}$ , FT-IR, UV absorption, photoluminescence (PL), and cyclic voltammetry (CV). The thermal properties of this material were confirmed by using the thermogravimetric analysis (TGA) and differential scanning calorimeter (DSC).

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발표종류: 포스터, 발표일시: 목 10:30~12:30

## A High Triplet Energy Host Material for Organic Light Emitting Diode

유승진, 박현태, 오대환, \*권순기, 김윤희

경상대 화학과 \*경상대 나노신소재공학부

Organic light-emitting diodes (OLEDs), getting the spotlight as a next generation display spends less electric power compared with other displays, and it is the most suitable display for realizing flexible display, if it has high efficiency, quick response speed and wide viewing angle. The material was characterized by  $^1\text{H-NMR}$ ,  $^{13}\text{C-NMR}$ , FT-IR, UV absorption, photoluminescence (PL), and cyclic voltammetry (CV). The thermal properties of this material were confirmed by using the thermogravimetric analysis (TGA) and differential scanning calorimeter (DSC).

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## Low-Temperature Preparation Method of Nanoporous TiO<sub>2</sub> film electrode for Flexible Dye-Sensitized Solar Cell

권도훈, 김영일, 윤용태

부경대 화학과

The use of flexible plastic substrates in the fabrication of dye-sensitized solar cell(DSSC) is very attractive in the view of cost-low mass production and installation. A key factor for substituting glass substrate with plastic is low-temperature ( $T_c$ ) film. We have prepared relatively robust nanoporous TiO<sub>2</sub> film on the conducting plastic substrates such as polyethylene terephthalate(PET)/ITO and polyethylene naphthalate(PEN)/ITO at the temperature lower than 150°C by utilizing sol mixture of TiO<sub>2</sub> nanoparticles and titanium tetra isopropoxide. Various dye-sensitized solar cells were fabricated with these TiO<sub>2</sub> film electrodes, standard Ru-dye, electrolyte solution and counter electrode using both conducting plastic and glass substrate. The photovoltaic performance of these DSSC was compared with conventional DSSC that was prepared by high temperature heat treatment.

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발표분야: 재료화학

발표종류: 포스터, 발표일시: 목 10:30~12:30

## Synthesis and Properties of Anthracene Derivatives for Organic Thin Film Transistors

신민기, 고혜진, \*박소민, \*\*강소희, \*\*김윤희, \*\*\*권순기

경상대 고분자공학전공 \*경상대 고분자공학과 \*\*경상대 화학과 \*\*\*경상대 나노신소재공학부

The anthracene derivatives for organic thin film transistors were synthesized by Sonogashira coupling reaction. The oligomers were characterized by  $^1\text{H}$  NMR and thermal properties were investigated by differential scanning calorimetry, thermogravimetric analysis. These oligomers showed high thermal stability with 5% weight loss at  $330\text{ }^\circ\text{C}$  and glass transition temperature at  $150\text{ }^\circ\text{C}$ . And their spectroscopic and electrochemical properties investigated by cyclic voltammetry, UV-vis, photoluminescence. These oligomers were fabricated into the device by solution process. The OTFT device of the oligomer showed a charge carrier mobility of  $0.01\text{ cm}^2/\text{Vs}$ .



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발표분야: 재료화학

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## Investigations on the Hybridization Properties of DNA-Gold Nanoparticle Conjugates and Their Applications

오주환, 이재승

고려대 신소재공학부

We have investigated the hybridization properties of DNA-gold nanoparticle conjugates under various conditions. We have discovered that the hybridization properties are affected dramatically by several parameters such as temperature and buffer salt concentration. We have further experimentally demonstrated the roles of each parameter in view of electrostatic interactions. Based on these studies, a diagnostic application has been designed and demonstrated.

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발표코드: I-MAT.P-288

발표분야: 재료화학

발표종류: 포스터, 발표일시: 목 10:30~12:30

## Preparation of nanocrystalline $\text{MgSb}_2\text{O}_6$ films and its application to dye-sensitized solar cell

장지연, 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 the DSSC. In this work, magnesium antimony oxide,  $\text{MgSb}_2\text{O}_6$  with trirutile structure was synthesized by low-temperature hydrothermal method. The crystallinity and average particle size of  $\text{MgSb}_2\text{O}_6$  was able to be controlled by the adjustment of reaction time and temperatures. The band gap and the flat band potential of  $\text{MgSb}_2\text{O}_6$  were estimated with UV-Vis reflectance measurement and cyclic voltametric, respectively. The DSSC which was assembled using the  $\text{MgSb}_2\text{O}_6$  photoelectrode and a conventional Ru-dye (N719) exhibited the overall light-electricity efficiency of 0.66 % with the short circuit current ( $J_{sc}$ ) of 5.02  $\text{mA}/\text{cm}^2$  and the open circuit voltage ( $V_{oc}$ ) of 0.38 V under illumination (AM 1.5, 100  $\text{mW}/\text{cm}^2$ ).

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발표분야: 재료화학

발표종류: 포스터, 발표일시: 목 10:30~12:30

## 수열합성법으로 제조한 $\text{YVO}_4:\text{Eu}^{3+}$ 적색형광체 나노입자의 VUV

### 여기 하에서의 발광특성

서정현, \*최성호, \*\*정하균

고려대 신소재공학과 \*한국화학연구원 소자재료연구센터 \*\*한국화학연구원 화학소재연구본부

최근 PID(Public Information Displays)의 부각에 따라 대형 스크린 및 투명 디스플레이에 대한 관심이 증폭되고 있다. 투명 디스플레이는 다양한 적용 분야가 거론되고 있는데, 건물 창문, 버스 및 지하철의 창문의 광고용 디스플레이에 적용이 가능할 것으로 기대되고 있다. 이러한 투명 디스플레이 제조에 플라즈마 디스플레이 방식이 적용될 수 있다. 본 연구에서는 투명 PDP에 적용할 목적으로 나노미터 크기의 형광체 입자를 제조하였다. 형광체는 hydrothermal 법을 사용하여 합성하였다. 147nm 진공 자외선 여기 조건에서 우수한 색좌표 특성을 나타내는 것으로 알려진 바나테이트계 화합물로서  $\text{YVO}_4$  모체에  $\text{Eu}^{3+}$ 을 활성제로 사용한 적색 형광체를 제조하였고 발광특성을 상용의 적색 형광체와 비교하였다. 또한, Nano-size 입자 생성을 위해 ethylene glycol (EG)을 첨가하여 microemulsion 상을 이용하였다. 생성된 나노입자의 형태와 크기를 FE-SEM 으로 확인하였다. Water 과 EG 의 비율에 따른 광발광 특성과 입자형태의 변화를 조사하였다. 합성된  $\text{YVO}_4:\text{Eu}^{3+}$  적색 형광체는 X 선 회절법에 의해 단일상 구조를 확인하였으며, 0.3ms 정도의 매우 짧은 잔광시간을 가짐을 알 수 있었다.

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발표종류: 포스터, 발표일시: 목 10:30~12:30

## 조성 변동에 따른 $\text{YAG:Ce}^{3+}$ 형광체의 진공자외선 여기 하에서의 발광 특성

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현재 주류를 이루고 있는 평판 디스플레이 중에서 PDP 는 응답 속도가 빨라 3 차원 디스플레이에 적용하기 유리한 것으로 알려져 있다. 3D 영상에서는 입체감을 크게 감소시키는 영상 중첩 현상을 방지하여야 하며 이에 따라 형광체는 4ms 이하의 짧은 잔광 시간이 요구된다. 하지만 기존의  $\text{Zn}_2\text{SiO}_4:\text{Mn}^{2+}$  녹색 형광체는 긴 잔광 시간을 가지므로 잔광시간을 감소시키기 위해  $\text{Y}_3\text{Al}_5\text{O}_{12}:\text{Ce}^{3+}$ 와 혼합하여 사용되고 있다. 본 연구에서는  $\text{Y}_3\text{Al}_5\text{O}_{12}:\text{Ce}^{3+}$  형광체에 있어 Al 자리에 Ga 의 치환, Al/Y 비의 변화 및  $\text{Ce}^{3+}$ 의 농도 변화와 함께 진공자외선 여기 하에서의 발광특성을 조사하였다.  $\text{YAG:Ce}^{3+}$  형광체들은 고상반응을 이용하여 1550℃에서 합성되었으며, 결정학적으로 단일상을 나타내는 것을 확인하였다.  $\text{Al}^{3+}$  자리에 이온 크기가 상대적으로 큰  $\text{Ga}^{3+}$ 의 치환으로 발광 스펙트럼의 중심 파장은 blue-shift 되었다. 형광체의 발광 강도에 근거하여 최적의  $\text{Ce}^{3+}$  농도와 Al/Y 비를 도출하였다. 또한, 진공자외선 여기 조건 하에서의 색좌표 변화와 잔광 시간 등을 측정하여  $\text{Zn}_2\text{SiO}_4:\text{Mn}^{2+}$  형광체와 비교하였다.

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발표코드: I-MAT.P-291

발표분야: 재료화학

발표종류: 포스터, 발표일시: 목 10:30~12:30

## **Noble method of boron carbide surface modification using epoxy resin**

전지현, 김재우, 엄영랑, 배연주

한국원자력연구원 원자력재료개발부

In the particulate composite system, the purpose of surface modification of fillers is to increase adhesion and dispersion of the fillers in the composite. In this study, the surface of boron carbide ( $B_4C$ ) particles was surface-modified by a noble method using epoxy resin. As starting material, mean- $0.5\ \mu m$   $B_4C$  particle was chosen. A hydrogenated type epoxy resin (ST3000) was used to form an epoxy coating layer on the surface of  $B_4C$ . The epoxy resin was dissolved into acetone, and subsequently,  $B_4C$  particles were added to the epoxy resin-acetone solution. To achieve uniform dispersion of  $B_4C$  particles, the epoxy resin-acetone solution containing  $B_4C$  was ultrasound-treated for 30min. After the ultrasound treatment, the solution with  $B_4C$  particle was placed at a drying oven to evaporate acetone solvent and collect a surface-modified  $B_4C$ . The surface morphology and diffraction pattern of  $B_4C$  particles with or without the surface modification were compared to confirm the presence of epoxy coating layer by means of FESEM (Field Emission Secondary Electron Microscopy) and XRD (X-ray Diffraction).

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발표코드: I-MAT.P-292

발표분야: 재료화학

발표종류: 포스터, 발표일시: 목 10:30~12:30

## Mass production of graphene flakes base on thermal plasma jet system

김주한, 서정쌍

서울대 화학부

We report the fabrication of graphene flakes composed of multi-layer graphene sheets in mass production base on thermal plasma jet system. A carbon atomic beam was generated by injecting  $\text{CH}_4$  gas into Ar plasma continuously; the beam then flowed through a carbon tube attached to the anode. Graphene flakes were made by epitaxial growth where a carbon atomic beam, having the proper energy, collided with a substrate. The production of large quantities of graphene flakes composed of graphene sheets will allow for the development of large-scale applications of this material.

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발표코드: I-MAT.P-293

발표분야: 재료화학

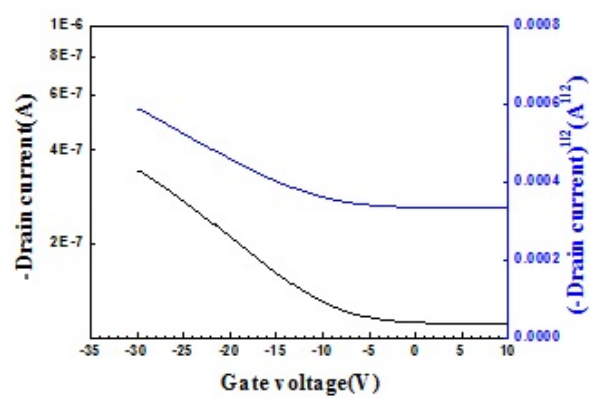
발표종류: 포스터, 발표일시: 목 10:30~12:30

## A New Type of Dragon-Fly shaped pyrrolo-perylene based on monothiophene polymer for OTFTs

**LU WANXIANG**, \*신민기, \*고혜진, 박소민, \*\*김윤희, \*\*\*권순기

경상대 고분자공학과 \*경상대 고분자공학전공 \*\*경상대 화학과 \*\*\*경상대 나노신소재공학부

A new kind of organic polymer based on monothiophene with alkyl end capping units was synthesized and fully characterized through proper structural design and instrument analysis. The synthesized pyrrolo-perylene based polymer(PLWX2) was characterized by the elemental analysis,  $^1\text{H}$  NMR, FT-IR. The thermal and photophysical properties of PLWX2 was also studied using thermalgravimetric analysis (TGA), differential scanning calorimetry (DSC), cyclic-voltametry (CV), UV-Vis absorption and photoluminescence (PL) studies. The band-gap of polymer is 2.03 eV and the HOMO is 5.27 eV. The large band gaps and low-lying HOMO energy levels could result in much better stability. The alkyl substituted end capping units enhanced solubility of the polymer in the organic solvents such as chloroform and dimethylchloride. Solution processed OTFTs (Top contact) based on PLWX2 as an active layer showed the higher field effect hole mobility of  $0.001 \text{ cm}^2 \text{ V}^{-1} \text{ S}^{-1}$ .





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발표분야: 재료화학

발표종류: 포스터, 발표일시: 목 10:30~12:30

## The New Quinary Thiophosphates with Interlocked Structures $A_3Nb_2Ti_2P_5S_{24}$ (A=Rb, Cs)

류재민, \*윤호섭

아주대 에너지시스템학부 \*아주대 화학과

The new quinary thiophosphates,  $A_3Nb_2Ti_2P_5S_{24}$  (A=Rb, Cs) have been prepared with the use of halide fluxes and the crystal structure of the compounds have been determined by single crystal X-ray diffraction method. The title compounds crystallize in the space group  $C_{2h}^6-C2/c$  of the monoclinic system with four formula units in a cell dimensions :  $a = 13.3326(4)\text{\AA}$ ,  $b = 27.3161(7)\text{\AA}$ ,  $c = 11.7834(4)\text{\AA}$ ,  $\beta = 116.1847(9)^\circ$ ,  $V = 3851.1(2) \text{\AA}^3$  for  $Rb_3Nb_2Ti_2P_5S_{24}$ ,  $a = 13.4219(4)\text{\AA}$ ,  $b = 27.5078(1)\text{\AA}$ ,  $c = 11.8079(4)\text{\AA}$ ,  $\beta = 116.0479(8)^\circ$ ,  $V = 3916.8(2)\text{\AA}^3$  for  $Cs_3Nb_2Ti_2P_5S_{24}$ . The structure of the title compounds are composed of octahedral  $TiS_6$ , tetrahedral  $PS_4$ , and bicapped trigonal prismatic  $Nb_2S_{12}$  units. The polyhedra form a three-dimensional framework by sharing S atoms. Two frameworks related by an inversion intertwine to complete the three-dimensional structure. However, there is no bonding interaction except the van der Waals forces between them. The charge balance of the compound can be represented by  $[A^+]_3[Nb^{4+}]_2[Ti^{4+}]_2[PS_4^{3-}]_5[S_2^{2-}]_2$ .

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장소: 제주ICC

발표코드: I-MAT.P-295

발표분야: 재료화학

발표종류: 포스터, 발표일시: 목 10:30~12:30

## **Assembly-Based Titration for the Determination of Monodisperse Plasmonic Nanoparticle Concentrations**

박현규, 이재승

고려대 신소재공학부

We present a stoichiometric titration method to determine the concentration of nanoparticles of various materials, sizes and shapes. Plasmonic nanoparticles and their assembly-dependent optical properties are used to monitor the assembly formation associated with their stoichiometry. We have discovered that assembly formation is maximized when two types of nanoparticles interact at specific ratios regardless of their sizes, materials and shapes. Based upon this observation, we titrate the particle of unknown concentration with high accuracy and efficiency using the reference particle whose concentration is known.

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발표종류: 포스터, 발표일시: 목 10:30~12:30

## The New One-dimensional Ternary Niobium Chloride Sulfide, $\text{Nb}_{24}\text{S}_{96}\text{Cl}_{16}$

이은실, \*윤호섭

아주대 에너지시스템학부 \*아주대 화학과

The new one-dimensional niobium chloride sulfide,  $\text{Nb}_{24}\text{S}_{96}\text{Cl}_{16}$  has been synthesized by using alkali metal halide fluxes and structurally characterized by single-crystal X-ray diffraction techniques. The title compound crystallizes in the space group P-1 of the triclinic system in a cell of  $a=16.7808(3)$  Å,  $b=19.8478(4)$  Å,  $c=19.8721(4)$  Å,  $\alpha=116.6754(7)^\circ$ ,  $\beta=97.6711(4)^\circ$ ,  $\gamma=94.5711(4)^\circ$ ,  $V=5788.0(2)$  Å<sup>3</sup>. The crystal structure contains three crystallographically independent chains. The chains have similar shapes and they are comprised of alternating long[3.5652(0)~3.6076(0) Å] and short[2.9216(7)~3.1393(7) Å] linear Nb-centered clusters made from five and three Nb atoms. Two kinds of Nb coordinations are observed in this compound. One of the terminal Nb atoms of the linear clusters is coordinated by three bridging disulfide ions ( $\mu_2$ ,  $\eta^2\text{-S}_2^{2-}$ ), ( $\mu_2$ ,  $\eta^1\text{-S}_2^{2-}$ ), and Cl<sup>-</sup>, whereas the others are surrounded by four ( $\mu_2$ ,  $\eta^2\text{-S}_2^{2-}$ ). There is no strong chemical bonding interactions, only van der Waals interactions among the chains. The UV/Visible spectrum of the compound shows an absorption edge and the band gap,  $E_g$  is estimated to be 1.26eV. The classical charge balance of the compound can be represented by  $[\text{Nb}^{4.5+}]_4[\text{Nb}^{4+}]_4[\text{S}_2^{2-}]_{16}[\text{Cl}^-]_2$ .

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발표분야: 재료화학

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## Flow chemistry를 이용한 Ionic liquids의 선택적 dication 합성

조원제, 이원길, 유국현

동국대 화학과

Ionic liquids (이하:ILs)는 상온 이온성 액체로 다양한 산업용매, 촉매, 열전달유체, 전지 전해질 등 다양한 사용처를 가지고 있다. 최근 들어 ILs 를 이용한 이차전지 전해질에 대한 연구가 활발해 지고 있다. 본 연구에서는 Ionic liquids 를 이용한 이차전지 및 커패시터용 전해질 개발을 위한 Ionic liquids 를 합성하기 위해 Flow chemistry 를 이용한 다양한 cation 유도체 합성을 시도 하였다. cation site 를 하나 갖는 ILs 에 대한 연구는 최근 들어 많이 이루어져 있다. 하지만 2 가지 이상의 cation site 를 가진 ILs 의 연구는 그리 많지 않아 새로운 전해질의 특성 연구를 위해 반드시 연구되어야 하는 필수 분야다. 본 연구에서는 다양한 dication ILs 를 합성하기 위해 micro loop 를 이용한 flow chemistry 방식의 합성법을 이용하여 효율적으로 dication ILs 합성을 시도하고 전해질 특성평가를 통해 dication site 에 따른 특성 변화를 관찰 하고자 한다.

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발표코드: I-MAT.P-298

발표분야: 재료화학

발표종류: 포스터, 발표일시: 목 10:30~12:30

## A Mechanistic Study on the Thermal Decomposition in Gadolinium Hydroxynitrate

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Gadolinium hydroxynitrate(GHN,  $\text{Gd}_2(\text{OH})_5(\text{NO}_3) \cdot x\text{H}_2\text{O}$ ) is a layered compound whose inorganic  $[\text{Gd}_2(\text{OH})_5]^+$  sheets include nitrate ions and water molecules in the gallery spaces. Due to its ion-exchangeable ability, GHN can intercalate much bulkier anions instead of losing nitrate ions. Thermal decomposition of GHN includes dehydration, dehydroxylation, decarbonation and denitration. In this study we suggest a decomposition mechanism of GHN from room temperature to 1000 °C with the help of XRD, FT-IR and TG-DSC-MS analysis. The GHN samples, heat-treated respectively up to 200, 300, 400, and 500 °C, still represent well-defined XRD patterns, nearly identical to those at room temperature. The thermochemical behavior shows that GHN is a good candidate as a catalyst support working nearly up to 500 °C.

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## Synthesis and growth of boron nitride nanotubes dependent on catalytic impurities during a milling-annealing process

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한국원자력연구원 원자력재료개발부 \*한국원자력연구소 원자력재료개발부 \*\*세종대 나노공학과

Boron nitride nanotubes (BNNTs) were synthesized and grown by using a mechanically activated boron powder. Mechanical activation energy transferred to boron powder during milling changes crystalline structure of boron to amorphous or disordered structure. Pulverization of boron powder was performed by using ball milling followed by annealing at  $\sim 1,100$  °C for nitration reaction of boron under nitrogen gas environment. Two different types of balls, zirconia ( $\text{ZrO}_2$ ) and tungsten carbide (WC), were used for milling producing different types of the catalytic impurities. Syntheses of  $\text{ZrB}_2$  and  $\text{W}_5\text{B}_2$  as well as BN during annealing were observed and dependent on the mechanical activation energy transferred to milled powder. Structural transformation of amorphous BN coat on the particle to the crystalline nanotube layers during annealing was observed using the TEM morphologies and confirmed by the EDX analysis. Consequently, the synthesis of BN and other chemical reactions of boron with nitrogen or other catalytic impurities during annealing were strongly dependent on the mechanical activation energy transferred to milled boron powder.

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발표코드: I-MAT.P-300

발표분야: 재료화학

발표종류: 포스터, 발표일시: 목 10:30~12:30

## The Synthesis and Structure of a New Mixed-metal Phosphates, $\text{Li}_x(\text{M/M}')_2(\text{PO}_4)_3$ ( $\text{M/M}' = \text{V/Nb}, \text{V/Ta}$ )

기용호, \*이승수, \*\*윤호섭

아주대 에너지시스템학부 응용화학과 \*나노정보융합기술연구소/아주대 \*\*아주대 화학과

$\text{Li}_3\text{M}_2(\text{PO}_4)_3$  have three structural phases: monoclinic  $\alpha$ -phase (below 120 °C), monoclinic  $\beta$ -phase (between 120 ~ 180 °C) and orthorhombic  $\gamma$ -phase (above 180 °C). The phase transitions among them are known to be reversible. We have prepared the orthorhombic phase of the mixed-metal phosphates,  $\text{Li}_{2.35}(\text{V}_{1.74}\text{Nb}_{0.26})(\text{PO}_4)_3$  and  $\text{Li}_{1.83}(\text{V}_{1.38}\text{Ta}_{0.62})(\text{PO}_4)_3$  as single crystals by the reactive alkali metal halide and structurally characterized by single-crystal X-ray diffraction techniques. They are isostructural and crystallize in the space group Pbnm of the orthorhombic system. The structures of the title compounds are comprised of (M/M')-centered octahedra and P-centered tetrahedra. In both phases, the metal sites are occupied by statistically disordered M/M' atoms. These polyhedra are sharing O atoms to form a three-dimensional framework with huge empty space.  $\text{Li}^+$  ions reside in this space to stabilize the structure through electrostatic interactions. The classical charge balance of the title compounds can be represented as  $[\text{Li}^+]_x[\text{M}^{3+}]_{2-y}[\text{M}'^{5+}]_y[\text{P}^{5+}]_3[\text{O}^{2-}]_{12}$  ( $\text{M} = \text{V}$  and  $\text{M}' = \text{Nb}, \text{Ta}$ ).

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장소: 제주ICC

발표코드: I-MAT.P-301

발표분야: 재료화학

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## Comparison of cellular effects of photocatalytic titanium dioxide nanoparticles

박희옥, 유미리, 강성규, 김연정, 양성익

경희대 응용화학과

Titanium dioxide ( $\text{TiO}_2$ ) nanoparticle is an important product for nanotechnology because of its high stability, anticorrosion, and photocatalysis. There are extensive concerns on the potential risks of  $\text{TiO}_2$  nanoparticle to human health and environment. Some forms at least may be genotoxic, photocatalytic, and/or carcinogenic. In this study, we have characterized the physico-chemical properties of commercially available photocatalytic  $\text{TiO}_2$  nanoparticle and compared to cellular effects in HaCaT Cells with or without photoactivation. The present study has shown that  $\text{TiO}_2$  nanoparticles are cytotoxic to HaCaT cells even in the absence of photoactivation. This effect became more pronounced in the simultaneous irradiation of UVA dependent on photocatalytic potential of  $\text{TiO}_2$  nanoparticle. We also found that the cytotoxicity and oxidative stress of  $\text{TiO}_2$  nanoparticles strongly depends on physico-chemical properties including structure (anatase, rutile, or mixture), or photocatalytic potency of  $\text{TiO}_2$  nanoparticles.



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## Characterization of Cytotoxicity of Silica Nanoparticles

강성규, 박희옥, 유미리, 김연정, 양성익

경희대 응용화학과

Nanotechnology is a highly promising molecular technology which may present a variety of hazards for environmental and human health. In this study, we investigated about the cytotoxicity and the mechanisms of action of by LUDOX® silicon dioxide (silica; SiO<sub>2</sub>) nanoparticles with three different types (different size, stabilizers, and coating materials) in human neuronal SH-SY5Y cell line. Various dosages were treated for 48 h and measured cell viability with MTT assay. Our results show that alumina coated SiO<sub>2</sub> nanoparticle, CL showed less cytotoxicity than AM and TM SiO<sub>2</sub> nanoparticles. In non-differentiated cells and retinoic acid (RA)-differentiating cells, the morphological changes were more obvious in AM and TM SiO<sub>2</sub> nanoparticles-treated cells than the CL SiO<sub>2</sub> nanoparticle-treated cells. Treatment of 48 h of CL, AM, and TM SiO<sub>2</sub> nanoparticles did induce DNA-double strand breaks in non-differentiated cells. On the other hand, only TM SiO<sub>2</sub> nanoparticle did induce DNA-double strand breaks in RA-differentiating cells. Also, TM SiO<sub>2</sub> nanoparticle induced G0-G1 phase arrest and apoptosis in RA-differentiating cells. Thus, this study suggests that CL, AM, and TM SiO<sub>2</sub> nanoparticles affect on neuronal cell systems through a variety of interruption to biological processes. Further studies on the mechanism to more clearly elucidate the SiO<sub>2</sub> nanoparticle induced neuronal cell death, as well as on the relationship between the physico-chemical properties of nanoparticles and their cytotoxicity are warranted to gain an understanding of the phenomenon of different sensitivities of various SiO<sub>2</sub> nanoparticles.

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## Highly Ordered Silver Nanodot Pattern : from Fabrication to LSPR Applications

유해욱

KAIST 생명화학공학과

Silver has been widely used for optical sensing and imaging applications which benefit from localized surface plasmon resonance (LSPR) in nanoscale configuration. Many attempts have been made to fabricate and control the silver nanostructure in order to achieve the high performance in sensing and other applications. However, fatal mechanical weakness of silver and lack of durability for oxygen rich condition have interrupted the manufacturing of reproducible and high-throughput nanostructures using the top-down lithography approach. In this study, we suggest a steady fabrication strategy to obtain highly ordered silver nanopatterns that is able to provide tunable LSPR characteristic and high performance in optical sensing system. By using protecting layer of platinum on silver surface for dry lithographic etching process, we successfully obtained large-area silver nanopatterns with high reproducibility. The large-area silver nanopatterned structures were capable of enhancing Cy3 fluorophore labeled DNA signal.

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## Preparation of Fe<sub>3</sub>O<sub>4</sub>/TiO<sub>2</sub> core-shell particles using peptization method and their photocatalytic properties

정은구, 김정수, \*구상만

한양대 화학공학과 \*한양대 화학공학

Titania (TiO<sub>2</sub>) is a chemically stable and environmentally benign substance which exhibits several interesting properties. It has been generally known not only as a white pigment, but also as a UV protection reagent due to its high refractive index and strong absorption energy band at UV region. Recently, nano sized titania particles have received growing attention in field of photocatalyst, solar energy conversion, and environmental sensors. However, titania nanoparticle also exhibits some disadvantages such as difficulty to recollect after use. To improve their recoverability, ferromagnetic Fe<sub>3</sub>O<sub>4</sub> core-TiO<sub>2</sub> shell particles with controllable thickness and crystallinity were prepared using peptization process. This method can not only avoid the complicated processes such as a layer-by-layer technique and polymer/surfactant grafting methods, but also reduce the cost by a short reaction time and a use of inexpensive reactants. The crystallinity of titania nanocrystals coated on core-shell particles was controlled by adjusting the pH of reaction medium and the optimum conditions for the formation of core-shell particles were established by systematically changing the reaction variables such as concentration, temperature, and time. Photocatalytic properties of Fe<sub>3</sub>O<sub>4</sub>/TiO<sub>2</sub> core-shell particles were also evaluated by investigating the degradation of rhodamine B dye under UV and visible light irradiation.

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## **Syntheses of lead precursors with high thermal stability for FeRAM thin film**

**김정수, \*하정민, \*\*구상만**

한양대 화학공학과 \*한양대 수소연료전지공학과 \*\*한양대 화학공학

In general, thin films of PZT materials are prepared by a sputtering method. However, in order to get high density memory devices of PZT, chemical vapor deposition (or atomic layer deposition) method should be employed because it provides better step coverage. Various kinds of organometallic and inorganic precursors of Pb, Zr, and Ti have been developed for CVD/ALD processes. However, there has been a technical barrier in conventional Pb precursors because they are decomposed in too low temperature enough to maintain a desirable content of Pb in a thin film. Thus new types of Pb precursors having moderate thermal stability should be developed to solve this problem. Another method to solve the problem of high volatility of Pb is to use organometallic precursors containing both elements of Zr or Ti with appropriate molecular ratio in a single complex. In this study, we prepared new types of Pb complexes for PZT precursors and characterized their physical and chemical properties using XRD, IR, NMR, and etc. Their thermal properties for CVD/ALD process were also investigated with TGA-DSC analyses.

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## Synthesis of Hyper-branched Poly(amidoamine) Conjugated Hybrid Silica Particles for Metal Ions Chemosensors

하정민, \*정은구, \*\*구상만

한양대 수소연료전지공학과 \*한양대 화학공학과 \*\*한양대 화학공학

TMPyP( $\alpha,\beta,\gamma,\delta$ -tetrakis(1-methylpyridinium-4-yl)porphine p-toluenesulfonate) has been known as an excellent sensor material due to the stability and metal-binding capability. Despite of several merits of TMPyP molecules, the poor recyclability limits its independent and wide uses in practical application. In order to solve this recovery problem, several methods have been developed including grafting TMPyP molecule in metal oxide such as silica. However, these methods have usually suffered from time consuming, long and multistep, process. In this study, we prepared multi-functional hybrid silica (MHS) particles containing vinyl, amine, and thiol functional groups by the modified sol-gel process and oxidized SH groups in MHS particles to SO<sub>3</sub>H groups in order to introduce TMPyP molecules. Hyper-branched Poly(amidoamine) MHS silica particles for higher loading of TMPyP molecules were synthesized by Michael addition with methylacrylate (MA) and the amidation of ethylenediamine(EDA), alternately. These hyper-branched MHS particles are able to amplify the visible and spectroscopic signals for Cd ion sensing due to huge increase in TMPyP concentration. Bare, 3rd, and 5th generation MHS particles were prepared and used for investigation of their heavy ion sensing capability. IR spectroscopy and Electron Microscopy were use to characterize the particles preparation. Colorimetric method and UV-vis spectroscopy was used to investigate the detection capability of prepared MHS particles.

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## **CuIn<sub>1-x</sub>Ga<sub>x</sub>Se<sub>2</sub> and CuSn<sub>0.5</sub>Zn<sub>0.5</sub>Se<sub>2</sub> thin film solar cells prepared by non-vacuum processing**

정재훈, 최선의, 김승주

아주대 에너지시스템학부

Non-vacuum depositions of CuIn<sub>1-x</sub>Ga<sub>x</sub>Se<sub>2</sub> (CIGS) thin film, a light absorption layer in solar cell, have attracted attention because of their simplicity in process and cost competitiveness. In this work, a simple non-vacuum process is proposed for fabrication of CIGS film. We attained amorphous colloidal precursors through ball-milling starting materials – elemental Cu, In, Ga and Se powders – in presence of liquid medium. We prepared the CIGS film by spin-coating the precursor on Mo substrate and then examined crystallinity by X-ray diffractometer. As indium was substituted by gallium in CuIn<sub>1-x</sub>Ga<sub>x</sub>Se<sub>2</sub> thin film, lattice parameter gradually decreased. The increment of bandgap from 1.03 eV to 1.50 eV was observed as Ga amount (x) increased from 0.0 to 0.7. As a simple and less-toxic preparative route, this method would be applicable to other absorption layers such as CuSn<sub>0.5</sub>Zn<sub>0.5</sub>Se<sub>2</sub> (CTZS) as well as CIGS.

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## Three-dimensional structured polyanilines.

연주랑, 신구, SINGH VIVEK KUMAR, 한승현

세종대 화학과

Polyaniline, a conducting polymer, has received great research interest because of its excellent electronic and chemical properties. A great number of one-dimensional structured polyanilines such as nanofibers have been studied but few literatures report about the three-dimensional structured polyanilines. In this study, we have developed a synthesis route for three-dimensional polyanilines such as open hollow sphere, hollow sphere, and sea urchin-like sphere by a self-assembly method, which are confirmed by SEM images.

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## Organic polymer coatings on Supper-hydrophilic coated surface for increasing the surface hardness without changing of surface wettability

박상수, \*이상균, \*\*최선, \*\*\*황현, \*\*\*\*박형기

성균관대 생명공학과 \* (주)대흥기업 기술연구소 \*\* 성균관대 생명공학연구소 \*\*\* 성균관대 생명공학부 \*\*\*\* 한국생산기술연구원 생산자동화센터

In this study, the SiO polymer coating film was prepared the containing tetraethyl orthosilane (TEOS) solution by the sol-gel method on soda lime glass. After then, the plasma polymer coating was deposited on SiO polymer coated glass by plasma enhanced chemical vapor deposition (PECVD) method at room temperature during 15 seconds. The thiophene monomer was used as organic precursor. It was heat up to 60 oC and bubbled with hydrogen gas which flow rate was 50 sccm. Plasma was ignited by radio frequency (RF, 13.56 MHz) and its power was 10 W. SiO polymer and plasma polymer coated SiO polymer films were investigated by Fourier Transform Infrared (FT-IR), scanning electron microscopy (SEM), ultraviolet-visible (UV-Vis.), water contact angle, the adhesion test, and the pencil hardness test. The IR spectra shows evidence of very thin organic plasma polymer, which could not be measured by SEM cross image. The SEM images show that the morphology of each film was not changed by plasma polymer coating. Low water contact angles showed with both coating. Moreover surface hardness was increased by plasma polymer coating.



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## Synthesis and Characterization of Polyimide-SiO<sub>2</sub> Nanocomposites by Surface Modification of SiO<sub>2</sub>

김영재, 이진규

서울대 화학부

Polyimide-SiO<sub>2</sub> nanocomposites were successfully prepared by surface modification of silica nanoparticles with a ligand that has a structure similar to that of polymer repeating units. The modified silica nanoparticles in poly(amic acid) solution were subject to thermal imidization to obtain polyimide-SiO<sub>2</sub> nanocomposite films. TEM analysis show that no significant aggregation in all polyimide-SiO<sub>2</sub> nanocomposite films having up to 30 wt% of silica nanoparticles. Prepared composites were characterized by Fourier-transform infrared (FT-IR) spectra, thermal gravimetric analysis (TGA) and transmission electron microscopy (TEM). It is expected that these polyimide-SiO<sub>2</sub> nanocomposite films exhibit improved mechanical and thermal properties in comparison with those of polyimide film itself.

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## **Facile Surface Modification of 3-Dimensional Polycaprolactone Scaffold for Enhanced Cellular Behaviors**

조선애, 이해신

KAIST 화학과

The research of 3-dimensional (3-D) scaffold has been extensively investigated as the importance of the 3-D scaffold increased in tissue engineering. 3-D scaffold offers the necessary support for cells to proliferate and maintain their biological functions. Furthermore, its architecture defines the shape of the new bone and cartilage growth. Polycaprolactone (PCL) has been of interest as a material of 3-D scaffold for tissue engineering, because of its excellent mechanical property and biocompatibility. However, there are practical problems for using it, in vitro and in vivo; extracellular matrix components and nutrients cannot penetrate into the inner space of scaffold, due to its hydrophobic property, and thus cell seeding and attachment onto the inner surface remain as a challenge. Thus, the surface modification strategy of 3-D PCL scaffold is a critical prerequisite for successful tissue engineering. Herein, we utilized a mussel-inspired approach for surface modification of 3-D PCL scaffold. Modifications of 3-D PCL scaffolds were carried out by simple immersion of scaffolds into the dopamine solution and stimulated body fluid, and as a result, hydroxyapatite-immobilized 3-D PCL scaffolds were obtained. The wettability of 3-D PCL scaffold was significantly changed after surface modification, and infiltration of the pre-osteoblastic cells into the 3-D scaffold followed by the attachment onto the surface was successfully achieved.

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## **Fabrication of N-type Flexible Semiconductor Using Molecular Layer Deposition Combined with Atomic Layer Deposition**

한규석, \*권덕현, 성명모

한양대 화학과 \*한양대 자연과학대학 화학과

We report a high-performance and air-stable flexible and invisible semiconductor which can be substitute for the n-type organic semiconductors. N-type organic-inorganic nanohybrid superlattices were developed for active semiconducting channel layers of thin film transistors at low temperature of 150 °C by using molecular layer deposition with atomic layer deposition. In these nanohybrid superlattices, self-assembled organic layers (SAOLs) offer structural flexibility, whereas ZnO inorganic layers provide the potential for semiconducting properties, and thermal and mechanical stability. The prepared SAOLs-ZnO nanohybrid thin films exhibited good flexibility, transparent in the visible range, and excellent field effect mobility ( $>7\text{cm}^2/\text{V}\cdot\text{s}$ ) under low voltage operation (from -1 to 3V). The nanohybrid semiconductor is also compatible with pentacene in p-n junction diodes.

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## Gels for Decontaminating Surface

방인배, 배봉문, 박윤봉

충남대 화학과

Decontamination gels have potential applications to remove radioactive or bio-hazard materials on the surface. The gels can be brushed or sprayed onto the contaminated surfaces as solution. That's why they can be applied easily to the areas that are not reachable by hands otherwise. After drying, gels can easily be removed from the surface. The gel is composed of colloidal solution containing a surfactant and an inorganic viscosifier. The gel has the property of thixotropy; a lower viscosity when stirred at a high speed and a high viscosity when stirred at a slow speed. The gel can be sprayed onto the contaminated surface and adhere easily to the surface. The gel's thixotropy depends on relative amount of inorganic viscosifier and surfactant to the total weight of gel. We have studied gels formulated from CAB-O-SIL M-5 fumed silica and nonionic surfactants of diethylene glycol hexyl ether, tripropylene glycol butyl ether, or tripropylene glycol dodecyl ether. Various compositions, by controlling the relative amounts of CAB-O-SIL M-5 fumed silica and adding various types of surfactants, were evaluated prior to adding the decontaminants. The decontaminants can be selected specifically based on the nature of the contaminations at the time of the decontamination process. Here in this work, we like to report and compare the characteristics of the gels based on the cracking sizes, automatic detachment ratios upon drying, and the viscosity before and after the gel formation.

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## **Ionic conductivities measurements of solid electrolytes using electrochemical impedance spectroscopy**

김병기, 오규환, 박윤봉

충남대 화학과

Molten salt thermal batteries are activated by raising their temperature above the melting point of the salts constituting the electrolyte. Lithium halide-based mixtures were mainly used as electrolytes for their low melting points, low vapor pressure and their relatively high ionic conductivities. For the long-life thermal battery, the electrolytes are expected to have not only the low melting point but also the high ionic conductivity so it can conduct current without solidifying at relatively low temperature. In order to evaluate the ionic conductivity of electrolytes, a BN cell, which are stable at high temperatures and chemically inert, are to be used. We have designed a BN cell for this work and measured several electrolytes with novel compositions using electrochemical impedance spectroscopy (EIS). Their values were compared with the common electrolytes (LiF-LiCl-LiBr, LiF-LiBr-KBr) used in thermal battery applications and were shown that novel electrolytes exhibit interesting ionic conductivities, which is suitable as electrolytes in long-life thermal batteries. The physicochemical properties of electrolytes were also studied by thermogravimetric analysis (TGA), differential thermal analysis (DTA), differential scanning calorimetry (DSC) and X-ray powder diffraction (XRD).

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## Multifunctional nanoplatform for DNAzyme Delivery: Towards New Hepatitis C Drug

유수윤, 장홍제, \*김동은, 민달희

KAIST 화학과 \*건국대 생명공학과

Recent studies in gene therapies have shown the potential of DNAzyme (Dz) as therapeutics due to several advantages including cost-effectiveness, facile chemical modification and relatively high stability against serum both in cell-based assays and in preclinical models of diseases including cancer and viral infectious diseases. A particularly important challenge in achieving the successful down-regulation of gene expression is to deliver DNAzymes efficiently. Since various nanomaterials have unique, useful chemical, physical, and mechanical properties, they can be used for a wide variety of applications including nano-based biosensors, drug delivery devices, diagnostic tools, and means for tissue engineering and fundamental cell biology studies. In this report, we describe synthesis and characterization of multifunctional magnetic nanoparticles (MION) that are designed for both noninvasive in vivo imaging and delivery of DNAzyme to target organ for hepatitis C treatment. We believe that our DNAzyme delivery platform will be one of the widely applicable and acceptable therapeutic options for the efficient HCV treatment in near future.

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## Crystal structure and ionic conductivity of Li-containing rare earth polyphosphates

이미선, 김성철, 김승주

아주대 에너지시스템학부

A series of lithium rare earth polyphosphates,  $\text{LiLn}(\text{PO}_3)_4$  ( $\text{Ln}$  = rare earths) have been synthesized by conventional solid state reaction. The crystal structure of the compounds was determined from the powder X-ray diffraction data. It crystallizes monoclinic system with space group  $C2/c$  and  $Z = 4$ . The lattice of  $\text{LiA}(\text{PO}_3)_4$  is built of twisted zig-zag chains running along with the b-axis and make up of  $\text{PO}_4$  tetrahedra sharing two corners, connected to the  $\text{LnO}_8$  and  $\text{LiO}_4$  polyhedra by common oxygen atoms to form a three-dimensional framework. The thermal behavior and the ionic conductivity of these compounds were measured by impedance spectroscopy. Furthermore, the correlation between crystal structure and ionic conductivity was studied.

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## **Fabrication and Characterization of CdSe/ZnS Quantum Dots and Polystyrene-Azide-Thiol(PS-N<sub>3</sub>SH) Polymer Composite Thin Films**

홍성표, \*도영락

국민대 생명나노화학 \*국민대 생명나노화학과

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. The QDs-polymer composite thin films(PS-N<sub>3</sub>-SH-QDs) were prepared by an photocross-linking process of spin-coated thin films using the photocross-linkable polystyrene with azide(N<sub>3</sub>) and thiol groups(-SH) for capping ligands of QDs. The PS-N<sub>3</sub>-SH-QDs thin films are characterized by PL spectroscopy, UV-vis, FE-SEM, AFM.



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## **The size effect of nanocrystalline surface scattering on the enhanced light extraction from 2D photonic crystal assisted $\text{Y}_2\text{O}_3:\text{Tb}^{3+}$ thin-film phosphors**

오정록, 박병규, \*도영락

국민대 화학과 \*국민대 생명나노화학과

Thin-film phosphors (TFPs) suffer from low external efficiency because of their low extraction efficiency, which arises from the total internal reflection (TIR) at the interface with a significant difference in refractive index. This is well known as the wave-guiding effect. In general, if emission is measured from only one surface and light propagating towards the substrate is not reflected, only 6.7% ( $n = 1.93$ ) of the light lies within the cone for a smooth  $\text{Y}_2\text{O}_3:\text{Tb}^{3+}$  thin film. We describe the effects of the grain size of sol-gel derived nanocrystalline  $\text{Y}_2\text{O}_3:\text{Tb}^{3+}$  TFPs on the enhancement of the extraction efficiency of emission light and the absorption of UV excitation light caused by Bragg scattering from over-coated two-dimensional (2D) polystyrene (PS) photonic crystal layer (PCL).

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발표종류: 포스터, 발표일시: 목 10:30~12:30

## **Fabrication of Multifunctional TiOx nanostructure; On Applying Neural Electrode & Bioscaffold**

김용희, \*이봉준, 백남섭, \*\*정명애, 정상돈

한국전자통신연구원 신경계인터페이스연구팀 \*한국전자통신연구원 융합기술연구부문 BT융합부 \*\*한국전자통신연구원 신기능정보소자팀

We have fabricated the TiOx nanostructure on transparent conducting plate by low temperature hydrothermal reaction and investigated the application possibility as a material for neural electrode and bioscaffold. TiOx nanostructure was fabricated through a simple hydrothermal reaction of alkali with the TiOx precursor-coated indium-tin oxide substrate. The electrochemical impedance spectroscopy (EIS) showed that the impedance of TiOx nanostructure is lower than that of TiOx film. And also neuronal cells are grown on both TiOx nanostructure and TiOx film. It was obvious that the cell morphology is more homogeneous and uniform on TiOx nanostructure while the cells on TiOx film forms cluster. These results suggest that the TiOx nanostructure could be potentially useful as a material for neural electrode and bio-scaffold.

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## **Luminescent properties of InP/ZnS quantum dots by a solvothermal method**

박병규, \*이경남, \*\*도영락

국민대 화학과 \*국민대 생명나노과학부 \*\*국민대 생명나노화학과

InP quantum dots (QDs) were synthesized by a solvothermal method via the pyrolysis reaction between indium chloride and greener phosphorus source of tris(dimethylamino)phosphine instead of highly toxic  $\text{P}(\text{TMS})_3$  widely used, at relatively low temperatures ( $150^\circ\text{C}$ – $180^\circ\text{C}$ ). The InP QDs after size-selective precipitation had a well-crystallized zinc blende structure, a narrow size distribution, and distinguishable absorption peaks. While as-grown InP QDs showed an undetectably low emission intensity, post-synthetic treatments such as ZnS shell coating gave rise to a substantial increase in emission efficiency due to the effective passivation of surface states. The resulting InP/ZnS core/shell QDs, emitting from blue to red wavelengths, and their luminescent properties (emission bandwidth and quantum yield) were comparable to Rhodamine 101 dye

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## Improvement of efficiency and color purity of amber monochromatic pc-LEDs combined with nano-multilayered optical filter

오지혜, \*오정록, 도영락

국민대 생명나노화학과 \*국민대 화학과

We studied amber monochromatic phosphor-converted light-emitting diodes (pc-LEDs) using a InGaN blue LED and a nano-multilayered optical filter (long-wave pass filter, LWPF), which is blue reflecting, amber passing filter, to overcome color mixing (low color purity) and difficulty of achieving reasonable efficiency for emission in the deep green to amber region of spectrum between 510 -610nm of III-V-based monochromatic semiconductor LEDs. The LWPF enhances the amber emission from the (Sr,Ba,Ca)<sub>3</sub>SiO<sub>5</sub>:Eu phosphor layer and color purity by blocking and recycling of the pumping blue light. The amber monochromatic pc-LEDs were fabricated by simply capping a LWPF on top of pc-LEDs. The optical properties and current/temperature stability of LWPF-capped amber pc-LEDs were measured to confirm the external efficiency and color purity. The enhancement of the luminous efficacy of the amber pc-LED with a LWPF (phosphor concentration 20 wt%, 39.4 lm/W) is 34% over that of an amber pc-LED without a LWPF (phosphor concentration 55 wt%, 29.4 lm/W) at 100 mA and a high color purity (> 96%) with Commission International d'Eclairage (CIE) color coordinates of x = 0.57 and y = 0.42.

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발표분야: 재료화학

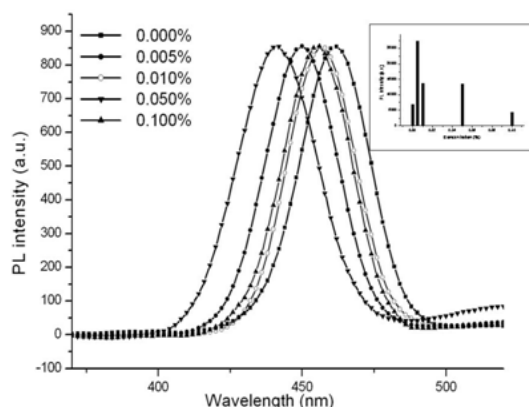
발표종류: 포스터, 발표일시: 목 10:30~12:30

## Synthesis and photoluminescence of Mg, Cu-doped CdS/ZnSe QDs

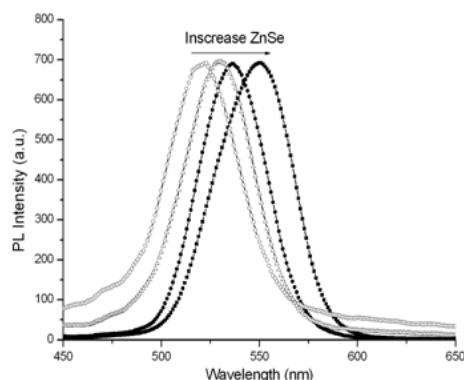
buithehuy, 서민호, 임재민, 이용일

창원대 화학과

Magnesium or copper-doped CdS/ZnSe (core/shell) nanoparticles were synthesized by direct solution of chemical routes in the organic solvent. XRD pattern confirmed the single phase and the mean size of nanoparticles was 3-4 nm by TEM. The Mg or Cu-doped CdS shows the obvious blueshift due to the replace of Cd by Mg or Cu ions. However, the concomitant presence of Mg and Cu, emission peak positions relatively shift to red range in comparison with Cu-doped CdS and the photoluminescence (PL) intensity of CdS:Mg,Cu/ZnSe was higher than that of the undoped CdS and CdS/ZnSe. Mg and Cu ions can be played the role of energy transfer centers because the shape of PL spectra did not change with Mg or Cu doped into CdS/ZnSe. These dopants are suggested as a simple and effective way to control their emission color of CdS/ZnSe nanocrystals. Keywords: blueshift, Mg, Cu, CdS/ZnSe, photoluminescence.



Dependence of PL intensity of CdS:Mg,Cu with varied concentration of Cu at 0.2% Mg



Effect of thickness of ZnSe on emission wavelength

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## Synthesis and Characterization of Green Phosphorescent Iridium(III) Complexes Derivative Phenylpyridine.

김철영, 강소희, \*신민기, \*\*권순기, 김윤희

경상대 화학과 \*경상대 고분자공학전공 \*\*경상대 나노신소재공학부

Organic light-emitting diodes (OLEDs) have attracted great attention in the past decades because of their potential advantages in full-color displays. In particular, phosphorescent metal complexes have been considered to be promising materials because of their ability to achieve maximum internal quantum efficiency, nearly 100%, as well as high external quantum efficiency in OLEDs. In this research, we report the synthesis of iridium complex using derivative phenylpyridine ligand. For the development of green phosphorescent Iridium(III) complexes, we led to a little blue shift from Ir(ppy)<sub>3</sub>. Therefore, the Iridium(III) Complexes Derivative Phenylpyridine moieties would be expected to be the best way to achieve an efficient phosphorescent emitter. The result of, we were characterized the structure of material, thermal properties and electrochemical properties.

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## Enhanced extraction efficiency of $\text{Y}_3\text{Al}_5\text{O}_{12}:\text{Ce}^{+3}$ ceramic phosphor using 2D photonic crystal

박후근, \*오정록, 성형철, 도영락

국민대 생명나노화학과 \*국민대 화학과

We propose the addition of two-dimensional (2D)  $\text{SiO}_2$  photonic crystal layer (PCL) on top of  $\text{Y}_3\text{Al}_5\text{O}_{12}:\text{Ce}^{+3}$  (YAG:Ce) ceramic phosphor to achieve enhanced extraction efficiency of ceramic phosphor on top of a blue InGaN light-emitting diode (LED) cup with the aim of achieving high-efficiency white LED. The low external efficiency of YAG:Ce ceramic phosphor is due to poor light extraction efficiency by the total internal reflection (TIR) and waveguide effect. To reduce the TIR and the waveguide effect, 2D triangular-lattice air-hole nanoarrays of  $\text{SiO}_2$  as PCL were fabricated on the YAG:Ce ceramic phosphor by nanosphere lithography (NSL). YAG:Ce ceramic phosphor with three different thicknesses (0.1, 0.2, 0.3mm) were used to analyze the enhanced light extraction efficiency by change of ceramic phosphor thickness. The structural, morphological and optical properties of YAG:Ce ceramic phosphor on top of a blue LED cup were investigated by performing scanning electron microscopy (SEM), atomic force microscopy (AFM) and photoluminescence (PL) measurements.

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## **Biomimetic Silicification of Amino acid-Functionalized Gold Nanoparticles for Formation of Nanocomposites**

이준오, 박지훈, 최인성

KAIST 화학과

The encapsulation of individual nanoparticles has attracted a great attention as a method for stabilizing nanoparticles and tailoring their surface properties. The encapsulation of nanoparticles with silica shells is especially advantageous for bioconjugation and applications to nanobiotechnology.<sup>1</sup> However, current chemical approaches toward silicification of nanoparticles generally require harsh reaction conditions. In this work, we suggest a new mild method for constructing amino acid-functionalized gold nanoparticle (AuNP)/silica core/shell hybrid structures by biomimetic silicification. The procedure consists of two steps: immobilization of amino acid-functionalized thiol ligands onto AuNPs and biomimetic silicification by tetramethylorthosilicate (TMOS). We believe that the method would provide a new route to the formation and applications of nanoparticle-based hybrid materials and composites.



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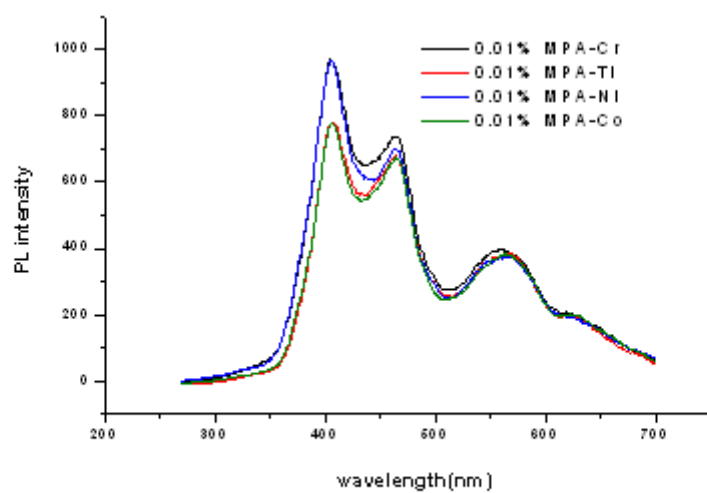
발표종류: 포스터, 발표일시: 목 10:30~12:30

## Effect of surfactant and transition metal Cr, Ni, Co, Ti -doped water-based ZnSe nanoparticles on the optical properties

서민호, buithehuy, 임재민, 이용일

창원대 화학과

The aqueous synthesis of ZnSe nanocrystal that implements low reaction temperature, low toxicity and water-soluble products has attracted more attention in recent years because of toxicity of cadmium chalcogenide (CdS, CdSe and CdTe) for human health. ZnSe quantum dots are doped with transition-metal (TM) ions and excited by UV light. It exhibits photoluminescence in the visible region with the color depending on the TM ion dopant. Surfactant ligands are MPA (3-mercaptopropionic acid), TGA (thioglycerol), MPS ((3-mercaptopropyl)trimethoxysilane), and glycerin as surfactants, which could not only reduce toxicity of QDs, but also overcome intrinsic disadvantages of limited QDs properties. TM-doped ZnSe nanocrystals with above surfactants have been directly synthesized in aqueous media. This study describes the synthesis of TM (Ni, Cr, Co, and Ti)-doped ZnSe nanocrystals from  $\text{Zn}(\text{NO}_3)_2 \cdot 6\text{H}_2\text{O}$  and Se by using surfactants, namely MPS, MPA, TGA, and thioglycerol in air atmosphere and aqueous media. The experimental variables including precursors and surfactant amounts had significant influence on the PL properties of the ZnSe nanoparticles. The optical features and structure of the TM-doped ZnSe quantum dots have been characterized by UV-vis, PL spectroscopy, TEM, and XRD. Keywords: transition metals, ZnSe, surfactants



PL emission spectra water-based ZnSe with surfactant and transition metal<sup>43</sup>



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## Highly Efficient Deep Blue-Emitting Material Based on Asymmetric Anthracene Derivative

김란, \*박현태, \*김철영, \*\*권순기, \*김윤희

경상대 화학교육과 \*경상대 화학과 \*\*경상대 나노신소재공학부

The anthracene derivative has received much attention due to their potential applications in OLEDs. For full-color displays, it is essential to have the three primary colors, red, green, and blue. However, compared with green-light-emitting devices, the EL properties of blue-emitting ones need to be improved, particularly in terms of efficiency and color purity, for full-color applications. Excellent blue-emitting materials are important, not only as blue emitters, but also as hosts for dopant emitters to facilitate efficient green and red emission. In this study, we designed and synthesized the anthracene derivative as a high twisted deep-blue light emitter. The structure of the anthracene derivative was confirmed using FT-IR, <sup>1</sup>H-, <sup>13</sup>C-NMR, and mass spectroscopy. In addition, this material characterized using electrochemical and physical chemistry methods. The electrochemical and photophysical properties of the new blue emitting material were also characterized. From the results, the anthracene derivative is a promising candidate for highly efficient deep blue-emitting material of OLEDs.

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## Superhydrophobic surface coatings via combinational use of perfluorinated xerogels and silica particles

윤종해, 송재훈, 신재호

광운대 화학과

Non-wettable surfaces with high water contact angles (so-called superhydrophobic nature) have received tremendous attention in recent years. Numerous studies have confirmed that combination of micrometer-scale and nanometer-scale roughness, along with a low surface energy material leads to apparent contact angle  $>150^\circ$ , a low sliding angle and the self cleaning effect. Various methods have been proposed to fabricate superhydrophobic surfaces mimicking the lotus surface structure, including lithographic patterning, plasma etching, electrochemical deposition, chemical vapor deposition, and layer-by-layer assembly. These methods often require harsh synthetic conditions and complex fabrication techniques, thus limiting the substrate type and geometry that may be coated. Herein, we describe synthesis of superhydrophobic surface coatings via combinational use of perfluorinated xerogels and silica particles. The effect of particle size on surface hydrophobicity is evaluated. A goniometer is used to measure the static contact angle and the surface morphology is also characterized using a scanning electron microscope (SEM) and atomic force microscope (AFM). Furthermore, the performance of spray coating and spin coating on surface hydrophobicity and stability is discussed. It is demonstrated that our synthesized superhydrophobic coatings can be easily applied to almost any substrates.

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## Facile Photopatterning Methods of Cell-Adhesive Polymer for Guided Neuronal Growth

백남섭, 김용희, 정상돈, \*정명애

한국전자통신연구원 신경계인터페이스연구팀 \*한국전자통신연구원 신기능정보소자팀

A facile microfabrication method was demonstrated via the photodegradation of cell-adhesive modified-poly(ethyleneimine) for guided neuronal growth. The photopatterned substrate was obtained by simple UV lithography process and plasma treatment of m-PEI coated on conducting electrode (ITO) or metal oxide surface. The biocompatible and micropatterned m-PEI layer can be used as support material in neuroelectronics to guide neurite outgrowth and control neurite extension of neuron. In this presentation, the details of various photopatterning methods and cell growth will be discussed.

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## Bio-inspired polymerization of DOPA and dopamine in presence of cysteine for generation of pheomelanin nanoparticles

표정, 황대웅, 이진규

서울대 화학부

멜라닌은 색소로 잘 알려진 생체 고분자로써 생체 여러 부위에 존재하며 광 보호, 항 산화 기능 등의 다양한 기능을 하기 때문에 여러 분야의 학문에서 관심의 대상이 되어 왔다. 멜라닌은 색에 따라 갈색의 eumelanin 과 붉은 색의 pheomelanin 으로 크게 나누어 진다. 일반적으로 eumelanin 은 tyrosine, DOPA, dopamine 등의 전구체를 효소적/화학적 산화 과정을 통해 인공적으로 합성할 수 있고, pheomelanin 은 cysteine 존재 하에 같은 반응을 진행 시켜 합성 할 수 있는 것으로 알려져 있다. 그러나 이전 연구들에서 발표한 인공적인 멜라닌들은 생체 내에 존재하는 천연 멜라닌과 같은 나노 수준 크기의 입자형태를 재현하지 못하여 입자형태에 기인한 여러 물리화학적 특성을 확인 하는 모델로 적합하지 않았다. 본 연구에서는 특정 산화제 및 염기 존재 하에 DOPA 및 dopamine•HCl 의 산화에 따른 중합반응으로 멜라닌 나노입자를 각각 합성하고 cysteine 존재 하에 같은 반응을 진행 함으로서 입자형태의 pheomelanin 모델을 합성 하였다. 만들어진 각각의 멜라닌 입자는 TEM(Transmission Electron Microscopy), ESR(Electron spin resonance), XPS(X-ray Photoelectron Spectroscopy), SAXS(Small Angle X-ray Scattering)를 통해 확인하였다.

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## Electrodeposited CdTe Thin film solar cell.

엄재호, 강바울, 이완인

인하대 화학과

CdTe thin film has many advantages because of its ideal band gap (1.45eV) and low-fabrication cost. In this study, solar cells of p-CdTe/n-CdS structure were prepared by electrodeposition of CdTe on Mo-coated glass. Molybdenum with thickness of 500 nm was prepared by Sputtering at 200°C. Three electrode systems were used for the electrodeposition of CdTe thin layer, While saturated calomel electrode (SCE) was used as a reference electrode and Pt Sheet as counter electrode. The Mo substrate was used as a working electrode for electrodeposition of CdTe layer in 3 hr in a bath containing CdSO<sub>4</sub> (0.5M) and TeO<sub>2</sub> (1×10<sup>-4</sup> M) at 30°C while its pH was adjusted to 1.8 and the deposition potential was set to be -300 mV to -600 mV versus SCE. After electrodeposition the CdTe/Mo layer was annealed at 400°C for 2 hr under argon environment in order to convert as-deposited n-type CdTe to p-type CdTe. CdS layer was assembled by chemical bath deposition method. The thickness of CdS layer was found to be 220 nm. Finally, AZO (aluminium doped zinc oxide) was sputter deposited. The photovoltaic properties of that fabricated Mo/CdTe/CdS/AZO thin film solar cell was analysed in this work.

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## 감마선을 이용한 코발트 수화물의 합성과 특성평가

박정훈, 허민구, 양승대, \*유국현

한국원자력연구원 방사선기기연구부 \*동국대 화학과

전극재에 쓰이는 코발트 수화물을 환원제 없이 감마선( $\text{Co-60}$ , 조사선량:  $24\text{KGy/hr}$ )만을 이용하여 합성하였으며 X 선 회절기(XRD), 주사전자현미경(SEM), 투과전자현미경(TEM)으로 구조와 표면분석을 통하여 나노크기의 3D-flower 형태의 이중층 구조임을 확인하였다. 전기화학적 특성을 알아보기 위해 순환전류법(cyclic voltammetry)과 임피던스 spectroscopy 를 통해 캐패시턴스 특성을 조사하였다. CV 결과를 통해 코발트 수화물의 산화환원 반응이 각각  $0.2\text{V}$ ~ $0.1\text{V}$  근처에서 나타남을 확인하였고 주사속도 5, 20,  $100\text{ m/s}$  에서 각각 246.7, 221.6,  $189.4\text{ F/g}$  의 비용량으로 보아 감마선을 이용하여 합성한 코발트 수화물의 특성이 우수한 전극재임을 알 수 있었다.



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발표코드: I-MAT.P-333

발표분야: 재료화학

발표종류: 포스터, 발표일시: 목 10:30~12:30

## **Structural relationship of melanin-like nanoparticles with photo-protection property**

주국연, 이진규

서울대 화학부

Melanins are well-known ubiquitous biological pigment relevant to various functions in bio-system such as photoprotection, antibiotic, thermoregulation, free radical quenching and some involvement in nerve systems. In particular, photoprotection property supported by a monotonically increasing absorption spectrum as a function of energy has been accepted as most prominent function of melanin in bio-system. Many structural models related to photoprotection mechanism have been suggested including oxidation, oligomerisation and stacking of proto-molecule of melanin. Especially, a wide range of aggregate sizes is known to be one of the most remarkable features of melanin and their natural tendency has been considered to be related with their photoprotective function. In this regard, three-dimensionally close packed structure of melanin-like nanoparticles were synthesized through neutralization of dopamine hydrochloride with NaOH followed by spontaneous air oxidation of dopamine. Through the precise investigation with photoluminescence spectroscopy, time-resolved fluorescence spectroscopy, high-resolution transmission electron microscopy and small angle x-ray scattering measurement, the structural relationship of melanin-like nanoparticles with photoprotection property will be discussed.

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발표종류: 포스터, 발표일시: 목 10:30~12:30

## **Ultralow dielectric constant pSiCOH films prepared with allyltrimethylsilane as skeleton precursor**

**박종민, \*공병선, 정희태**

*KAIST 생명화학공학과 \*KCC 중앙연구소*

Ultralow dielectric constant pSiCOH films have been prepared using allyltrimethylsilane(ATMS) as the skeleton precursor and a porogen precursor. The porogen has been removed from the deposited films by thermal annealing at 420 °C, obtaining films with dielectric constants down to 2.2. The films have been investigated by Fourier transform infrared spectroscopy, and n&k optical measurements of the refractive index (n) and the electrical characteristics have been measured on metal-insulator-semiconductor structures. It was found that the properties of the annealed films depend on the deposition temperature and concentration of porogen.

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## **Double coating of Au nanoparticles on single-walled carbon nanotubes (SWNTs) for transparent conducting films**

양승보, \*공병선, 정희태

KAIST 생명화학공학과 \*KCC중앙연구소

We investigated the electrical conductivities of single-walled carbon nanotube (SWNT) network films upon pre- and post-treatment via gold ions, particularly with respect to their potential use as transparent conducting films. Transparent conducting SWNT films using pre- and post-deposition of gold nanoparticles resulted in a significant decrease of the electrical resistance, while the initial value of the transmittance of pristine-SWNT films was maintained. The double Au nanoparticle hybrid films exhibited 5 times lower sheet resistance compared to pristine-SWNT films. The electrical behaviors of the gold nanoparticle-coated SWNT films were examined by an analysis of the work-functions of the SWNT films. The SWNT-Au nanoparticle hybrid films are expected to be applicable to transparent electrodes of various optoelectronic devices such as solar cells, light-emitting diodes, sensors, and field effect transistors.

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**Tissue engineering by protein adhesion & non-biofouling property :  
poly((3-(methacryloylamino)propyl)-dimethyl(3-  
sulfopropyl)ammonium hydroxide)**

최백합, 최인성

KAIST 화학과

Non-biofouling property is the most important in the field of tissue engineering. Poly((3-(methacryloylamino)propyl)-dimethyl(3-sulfopropyl)ammonium hydroxide), (poly(MPDSAH)) polymer has been studied highly efficient non-biofouling property. This work generated efficient non-biofouling polymeric thin film of (poly(MPDSAH)) from the self-assembled monolayers terminating in an initiator of atom transfer radical polymerization (ATRP) by the surface-initiated ATRP of MPDSAH. ATRP is one of the best methods for producing well-defined polymer brushes due to its versatility with respect to monomer type, its tolerance of impurities, and the typically mild reaction conditions. In this work, we described long term stability of poly(MPDSAH) under the protein condition. We utilized fibrinogen, lysozyme, ribonuclease A, and bovine serum albumin. The formed on the poly(MPDSAH) was observed to resist the protein adhesion up to for 25 days and confirmed ellipsometry, contact angle goniometry, and X-ray photoelectron spectroscopy.

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## **Drug delivery system based on the nano-hybrid material for the combinational therapeutics**

나희경, 민달희

KAIST 화학과

Mesoporous silica materials appear to possess immense potentials in catalysis, biosensors and drug delivery systems due to 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 biomaterials into mesopores, and for the retention of pore space after grafting of organic functional groups. In current research trend, nano-hybrid system has occupied an important position in the biomedical field because of its potential for creating the high performance by the combination of two or more nano materials overcoming the limitation of each material. Here, we report a drug delivery system based on the nano-hybrid material on the basis of pore expanded silica nanoparticle. The synthesis, characterization, and performance are discussed to prove the feasibility of the newly designed system. It is demonstrated that our system can serve as a safe and efficient therapeutic tool for the combinational approach of gene- and chemotherapy.

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## A New Platform for Endonuclease Activity Assay Based on Graphene Oxide.

이지언, 민달희

KAIST 화학과

Endonucleases, a family of nucleases that can hydrolyze the internal phosphodiester bonds in DNA or RNA, are one of the most important enzymes in molecular biology. They are responsible for many processes involving the replication, repair, and recombination of nucleic acids. Among them, restriction enzymes (type II) which cut DNA within their recognition sequences are frequently used in the laboratory for DNA analysis and gene cloning. Therefore, the assay of endonuclease activities is important in the fields of drug discovery, clinical diagnostics, and genetic engineering. Although the gel electrophoresis and isotope labeling are extensively chosen for endonuclease activity assay in most laboratories, they are generally time-consuming, discontinuous and not cost-effective. Recently, alternative approaches such as colorimetric and fluorescence method based on various nanomaterials have been developed for simple, real-time monitoring of endonuclease activity. In this report, we describe a new restriction endonuclease activity assay method based on the difference of binding affinity between single stranded DNA and double stranded DNA with GO. GO can be used as an efficient nano-quencher because it adsorbs single stranded DNA followed by long range energy transfer from dye. By measuring the quenching and recovery of fluorescence of dye conjugated to DNA substrate, endonuclease activity can be assayed. This GO-based method allows real-time measurement and quantitative assay of endonuclease activities in short time. We believe that this new GO based restriction enzyme assay platform will be a widely applicable tool in endonuclease related basic research and drug development.

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발표종류: 포스터, 발표일시: 목 10:30~12:30

## Preparation of Polyaniline Nanotubes by a Interfacial Polymerization Reaction

김지현, 신구

세종대 화학과

Nanotubes of conducting polyaniline(PANI) has electrical, electrochemical and optical properties coupled with excellent environmental stability like carbon nanotubes(CNTs). We have followed interfacial polymerization method to synthesize PANI nanofibers, in which aniline is chemically oxidative polymerized to PANI at the interface of two immiscible liquids. We have synthesized PANI nanotubes by using 1-Pyrenesulfonic acid(PSA) instead of dopant HCl.

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발표종류: 포스터, 발표일시: 목 10:30~12:30

## **Efficient gene delivery by using mesoporous silica nanoparticles with large pores providing high loading volume and protection of plasmid DNA**

김미희, 나희경, 김영관, 유수윤, 민달희

KAIST 화학과

Gene therapy has been an important research field to treat various genetic diseases such as cancer, hepatitis, and sickle-cell anaemia. The important prerequisite for successful therapy is efficient gene delivery system due to instability of nucleic acids under physiological condition and low permeability of nucleic acids to cell membrane. Therefore, continuous efforts have been devoted to apply various inorganic nanomaterials such as gold, iron oxide, carbon nanotube, quantum dot, and silica to gene delivery. These inorganic carriers are attractive candidates because of their long-term stability, amenable surface, and relatively high biocompatibility compared to viral carriers and cationic polymers. In this work, we developed efficient gene delivery system based on aminated mesoporous silica nanoparticles with large pores (> 15 nm). The mesoporous silica nanoparticles with large pores were successfully harnessed as a gene delivery carrier with high cellular uptake, biocompatibility, loading capacity, protection effect of plasmid DNA, and in vitro transfection efficiency of the luciferase and GFP (Green fluorescent protein) gene. To the best of our knowledge, this work is the first application of aminated large-pored mesoporous silica nanoparticles to gene delivery and we believe that this system will be a promising tool of other biomacromolecules delivery due to the large pores, high surface area, low cytotoxicity, cost-effectiveness, and simple synthetic and delivery process.



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## Synthesis of titania nanoparticle for enhanced photocatalytic approach

임주현, \*김준성, \*박수진, 이진규

서울대 화학부 \*(주)바이테리얼즈 부설연구소

Titania 는 고유의 다양한 특징 때문에 많은 분야에 이용되어왔고, 또 상당한 연구가 진행되고있다. Titania 의 고유한 흰색은 각종 염료로, 높은 UV 흡수력은 자외선 차단제로, 큰 dielectric constant 는 전기소자의 성능 향상에, 광촉매 능력은 오염물질 및 독소 제거에, 그리고 큰 bandgap 은 태양전지의 핵심 요소로 사용되는 등, 각각의 특징에 따른 응용이 활발히 진행되고 있다. 하지만 titania 는 전구체의 높은 반응성 때문에 균일한 크기의 입자로 합성하기가 쉽지 않다. 대부분 harsh 한 조건에서 입자를 합성하며, 그 결과물이 aggregation 되어 있거나, 다량의 surfactant 를 함유하고 있는 경우가 많다. Mild 한 조건에서 균일한 입자를 합성한 경우도 있지만 주로 그 크기가 200 nm 이상인 한계를 가지고 있다. 본 연구에서는 mild 한 조건에서, salt 또는 ethylene glycol 의 존재 하에 sol-gel method 를 이용하여 크기조절 가능한 구형 입자를 합성하였으며 그 크기를 60 nm 수준까지 줄이는데 성공하였다. 입자의 크기는 FT-SEM 및 TEM 으로 확인하였다. 특히 광 촉매 활성이 있는 anatase phase 를 만들기 위한 calcination 후에도 aggregation 되지 않았으며 그 결정성은 powder XRD 로 확인하였다. Anatase phase 의 입자는 UV 에서, 상용화된 P25 보다 좋은 광촉매 효과를 보였으며 유기염료의 degradation 실험을 통해 확인하였다. 또한 합성된 입자는 alkoxysilane compound 로 표면처리가 가능하며 FT-IR, DSC, 그리고 zeta potential 등을 측정하여 표면처리 결과를 확인하였다.

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## Quantificative analysis and efficient surface modification of silica nanoparticles

정학성, 문두식, \*김준성, \*정민숙, 이진규

서울대 화학부 \*(주)바이테리얼즈 부설연구소

하나의 아민 작용기를 갖는 3-aminopropyltrimethoxysilane (APTMS)와 세 개의 아민 작용기를 갖는 (3-trimethoxysilylpropyl)diethylenetriamine (DETAS)를 이용하여 실리카 나노입자의 표면을 재현성 있게 개질하였다. 이렇게 표면처리 된 실리카 나노입자의 표면에 존재하는 아민 작용기의 양은 산-염기 역적정법을 이용하여 정량하였고, 표면에 존재하는 아민 작용기와 형광 물질인 Rhodamine B isothiocyanate (RITC)와 반응시킨 후 UV-Vis 흡광을 통해 실제 반응에 참여하는 아민 작용기의 양을 정량하였다. 역적정을 이용해 얻은 아민 작용기의 개수는 SiO<sub>2</sub>-APTMS 와 SiO<sub>2</sub>-DETAS 에 대해 각각 2.7, 6.8 ea/nm<sup>2</sup> 의 아민기를 갖는다는 것을 확인할 수 있었으며, 형광 분자와의 반응 후 흡광을 측정한 결과 SiO<sub>2</sub>-APTMS(RITC)와 SiO<sub>2</sub>-DETAS(RITC)에 대해 각각 0.44, 1.3 ea/nm<sup>2</sup> 의 아민기가 RITC 와 반응함을 알 수 있었다.

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## **PCE enhancement of organic solar cell using simple nano-pattern methods**

최종길, 정희태

KAIST 생명화학공학과

Fullerene conjugated polymer based Bulk hetero-junction solar cell has been widely used over the last decade. and a lot of attention has been focused on engineering the properties of these system. there are varios methods to enhance power conversion efficiency like thermal annealing, surface patterning, optical spacer and co-solvent etc. In this study, regular nano pattern is successfully introduced on ther surface of active layer using simple soft lithography methods. It has been already reported that surface nano pattern can enhance the PCE of solar cell via scattering effect. but the change of phase separation and orientation of polymer chain during nano pattern was not fully understood. so In this work, surface nano pattern was introduced by different patterning methods ( thermal and solvent assisted molding ) then we investigated the phase separation and crystal orientaion using various characterization methods.

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## Enzyme immobilization studies on Mesoporous carbons supports and their applications

chaudhari kiran, \*김민식, \*김정호, \*\*송민영, \*\*\*양대수, \*\*김윤경, \*유종성

고려대 소재화학 \*고려대 신소재화학과 \*\*고려대 소재화학과 \*\*\*고려대 신소재화학

Immobilized enzymes on stable supports act as excellent catalyst in bio-sensors, biological catalysis and separations. Mesoporous carbons acts as excellent support for immobilization due it highly porous and inert nature and facilitate electron transfer due to its conductive nature. Recent developments in synthesis of mesoporous carbons have allowed excellent control over its morphology, pore size and surface area. Mesoporous carbons possessing high surface area with large mesopores act as an excellent support for immobilization of enzymes thus enhancing commercial values of important enzymes in terms of stability and productivity compared to other supports.

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## 스탬프용 레진의 광 경화 시간에 따른 기계적 특성 변화 연구

김주연, \*도이미

ETRI RFID/USN 소자자팀 \*한국전자통신연구원 원천기술연구부

Here we present mechanical properties of submicron patterned polyurethane acrylate (MINS-311RM, Minuta Tech., PUA) stamp that is fabricated by UV-imprint lithography. Mechanical properties were measured by the indented depth on PUA films during the loading-unloading cycles and recorded as a functional of the UV-exposure time by nanoindentation technique. Hardness and Young's modulus were increased up to 0.15 GPa and 2.7 GPa by increasing UV-exposure time which is indicating better mechanical properties according to highly crosslinked structure. These results are promising to get semi-permanent PUA stamp without any mechanical changes with time which is directly affecting for pattern transfer accuracy and its critical dimension.

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## **Fabrication of 2D TiO<sub>2</sub> nanoholes from TiO<sub>2</sub> nanoparticles by nanoimprint method**

최윤식, \*허은진, \*안진호, \*\*고기영

한양대 정보디스플레이공학과 \*한양대 신소재공학과 \*\*한국특허정보원

The 2-dimensional (2D) TiO<sub>2</sub> nanohole patterns have been prepared on various substrates by nanoimprint method. Nanoimprint process is based on the direct printing of a 2D nanoparticle patterns from a elastomeric stamp to a substrate. The elastomeric stamp was then imprinted into the substrate with a pressure of 10 atm at 100 °C for 1 hour. The sizes of the TiO<sub>2</sub> nanoparticles used in patterning 625 nm pitch were 50 nm. The pitch, diameter, and height of the TiO<sub>2</sub> nanopatterns were 625 nm, 325 nm, and 215 nm, respectively. The structural and morphological properties of 2D TiO<sub>2</sub> nanoparticle patterns were investigated and compared by performing X-ray diffraction (XRD), scanning electron microscopy (SEM) and atomic force microscopy (AFM).

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## Superparamagnetic Fe<sub>3</sub>O<sub>4</sub> Nanoparticles-Carbon Nitride Nanotube Hybrids for Highly Efficient Peroxidase Mimetic Catalysts

이정우, \*강정구

KAIST 신소재공학부 \*KAIST 신소재공학과

We report the facile route to synthesize size tunable Fe<sub>3</sub>O<sub>4</sub> nanoparticles (NPs)-carbon nitride nanotube(CNNT) hybrids. First of all, it is demonstrated that these NPs tunable with 2.3 nm to 7.9 nm sizes on CNNTs show the superparamagnetic values ranging from 2.58 to 15.95 emu/g. In addition, our densityfunctional theory calculations on two metallic and semiconducting CNNTs with (5, 5) and (8, 0)10 chiralities clarify that N PDOS near to the Fermi energy level are decreased as NPs anchor on N atoms of CNNTs, consistent with the decreased unoccupied N states from our experimental N K-edge near edge Xray absorption fine structure (NEXAFS). These imply that N atoms embedded on CNNTs provide selective anchoring sites for NPs. Also, it is found that the attached NPs on CNNTs were found to be on the uniform sizes without agglomeration observed in pure nanoparticle catalysts. In addition, these NPs-15 CNNT hybrids showing the water-soluble property are proven to give the ultra high peroxidase mimetic activity higher by about 60 times than those for pure magnetite NPs at the first 30 s, where a colorless peroxidase substrate 3,3',5,5'-tetramethylbenzidine changes by H<sub>2</sub>O<sub>2</sub> to its blue colored oxidized state.

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## 스티릴피라진계 색소의 고체상 압변/광변색 형광

문병천, 이왕은, \*곽기섭

경북대 고분자공학과 \*경북대 공과대학/고분자공학과

스티릴피라진계 유도체는 고체상에서 두 가지 결정상을 가지는 동질이상형 물질이다.1 본 연구에서는 이들 유도체가 글라인딩과 같은 기계적 자극에 의해 현저한 형광증대와 동시에 형광단파장이동을 관찰하였다. 뿐 만 아니라, 기계적 자극 후에 아주 약한 UV 광을 조사하면 더욱이 형광강도가 증대되는 것을 알았다. 우리는 형광분광분석, 형광현미분석, 편광현미분석, DSC 분석, X-ray 구조분석을 통해 고체상의 스티릴피라진계 색소들의 기계적자극과 UV 광자극에 의한 결정상전이 메커니즘을 규명하였고, 형광변화와의 연관성을 조사하였다.



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## Synthesis of functional core - fibrous silica shell particles with a tunable pore size

문두식, 이진규

서울대 화학부

기존에 알려진 섬유상 구조를 갖는 실리카 입자의 합성법을 개량하여 다양한 특성을 가지는 나노입자의 표면에 섬유상 실리카 껍질을 형성시킬 수 있었다. 반응물의 조성비를 달리하는 것만으로 기공의 크기를 수 nm 부터 수십 nm 까지 조절할 수 있었으며, 기존의 극초단파 오븐을 사용하는 방법 대신 환류법을 사용하여 보다 안전하고 쉽게 입자를 합성할 수 있었다. 상기한 합성법을 바탕으로 자성나노입자나 촉매활성을 가진 금속입자 등 다양한 기능성 나노입자를 핵으로 하여 섬유상 실리카를 껍질형태로 형성시킨 핵-껍질 구조의 나노복합체들을 합성하였다. 임의로 조절이 가능한 기공의 크기와 바깥쪽으로 갈수록 면적이 넓어지는 특유의 섬유상 구조는 특정 크기의 물질들이 왕래하기 용이하여 촉매나 약물전달, 단백질 및 입자의 선택적인 흡착 등에 좋은 효율을 제공할 것으로 기대된다. 상세한 합성과정과 이러한 나노입자들의 표면적과 구조를 이용할 수 있는 다양한 활용방안이 추후 논의될 것이다.

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## Synthesis of monodispersed $\text{Ln}^{3+}:\text{Gd}_2\text{O}_3$ nanoparticles for multifunctional imaging

유성민, 차진명, \*최제남, 이진규

서울대 화학부 \*서울대 화학과

최근 분자 또는 세포 수준에서 병리현상 등을 영상화하기 위한 시도가 이루어 지고 있고, 특히  $\text{Gd}_2\text{O}_3$  는 자성 특성을 통하여 MR 조영 효과뿐만 아니라, 다양한 기능을 가지는 f-오비탈의 란타나이드가 도핑될 수 있는 호스트 물질로 잘 알려져 있다. Urea-based thermal decomposition 에 의해 균일한 구형의 비정질 가돌리늄 산화물 입자를 합성하였으며, 농도 비율과 반응시간의 변화를 통해 입자의 크기를 50 nm 에서 200 nm 까지 조절할 수 있었다. 입자의 결정성을 증가시키기 위해 소결과정을 진행하였고, 소결과정 중 입자들의 뭉침 현상을 막기 위해 실리카 껍질을 형성시켰으며, 소결과정을 통하여 비정질의 구조가 입방 결정구조를 가지는  $\text{Gd}_2\text{O}_3$  를 얻었을 수 있었다. 또한 다양한 란타나이드를 도핑함으로써 형광과 자성을 동시에 가지는 다기능  $\text{Ln}^{3+}:\text{Gd}_2\text{O}_3$  나노입자를 합성할 수 있었다. 합성된 균일한 다기능  $\text{Ln}^{3+}:\text{Gd}_2\text{O}_3$  나노입자는 분산성, 안전성 등이 요구되는 다양한 바이오이미징 분야에 응용될 수 있을 것이다.

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## Effects of Cr<sub>2</sub>O<sub>3</sub> modification on the performance of SnO<sub>2</sub> electrode in DSSCs

최서영, \*권영욱

성균관대 화학 \*성균관대 화학과

Since the first dye-sensitized solar cell (DSSC) was invented, numerous studies have been performed to improve the efficiency of the cell. Surface modification, adding a small amount of semiconductor or insulator on the surface of the electrode material, is one of the strategies investigated. Several papers show that electrodes prepared from SnO<sub>2</sub> modified with other insulating oxides like ZnO and Al<sub>2</sub>O<sub>3</sub> have efficiencies superior to an electrode with tin oxide alone, because they have higher conduction band edges and are insulator. On the other hand, previously, we showed that semiconducting CdO can be a blocking layer because it has higher isoelectric point (IEP, IEP=10) than SnO<sub>2</sub> (IEP=4.5), deprotonating SnO<sub>2</sub>, so that increase open-circuit voltage, short-circuit current and efficiency. In this study, we choose Cr<sub>2</sub>O<sub>3</sub> as a surface modifier on SnO<sub>2</sub> nanoparticles because its IEP is 7, and its effects of Cr<sub>2</sub>O<sub>3</sub> on the performances of DSSCs are investigated as a function of Cr/Sn ratio. When Cr/Sn ratio was 0.02, 55%-improved overall conversion efficiency was measured and the ratio 0.05, 40% compared with pure SnO<sub>2</sub> cell. However, when Cr/Sn ratio was 0.20, the efficiency was very small because negatively charged SnO<sub>2</sub> could inject electron back to the electrolyte and result in recombination between photoelectrons and I<sup>3-</sup> in electrolytes. The other properties of Cr<sub>2</sub>O<sub>3</sub>-modified SnO<sub>2</sub> were studied by X-ray diffraction, capacitance measurement and electrochemical impedance spectroscopy.

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## **Dye-sensitized solar cells based on TiO<sub>2</sub> nanotube membranes filled with TiO<sub>2</sub> nanoparticles**

노철

서울대 화학부

We have fabricated dye-sensitized solar cells (DSSCs) based on TiO<sub>2</sub> nanotube membranes attached to fluorine-doped thin oxide (FTO) glass, whose channels were filled with TiO<sub>2</sub> nanoparticles. By filling approximately 10 wt% of TiO<sub>2</sub> nanoparticles to the membrane weight in the channels of the membrane, the energy conversion efficiency was enhanced from 5.2% to 6.3%, a 21% enhancement. By treating with TiCl<sub>4</sub> after filling with the TiO<sub>2</sub> nanoparticles, the efficiency was enhanced from 5.2% to 7.3% (a 40% enhancement) due to an increase in the total available surface area for dye adsorption. The combination of filling TiO<sub>2</sub> nanoparticles into the channels and then treating with TiCl<sub>4</sub> is a good method to improve the energy conversion efficiency of the DSSC based on TiO<sub>2</sub> nanotube membranes.

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## Simple preparation and low-cost iron oxide coated silica gel as adsorbent material for arsenic removal application

ARIFIN ERIC, \*차진명, \*이진규

서울대 나노과학기술정공 \*서울대 화학부

Arsenic contamination of surface and subsurface water has become global environmental issue as millions of people which have been exposed to contaminated drinking water develop severe health problems which call for proper treatment before its use as drinking water. Iron oxide coated silica gel was prepared using a simple, quick and reproducible method and its effectiveness for As(III) and As(V) removal was investigated by batch and column adsorption studies. Linear regression analysis showed that equilibrium adsorption data for As(III) and As(V) at different initial arsenic concentration and adsorbent dose of 50 g/L fitted Langmuir isotherm model with maximum adsorption capacity of 13.21 mg/g and 27.47 mg/g for As(III) and As(V), respectively. The results were also in agreement with those from column studies and are much larger than previously reported results on similar adsorbent-supporter system. Kinetic studies revealed that adsorption process was very rapid and could be well described by pseudo-second-order model. No pH or temperature adjustment was made during all adsorption experiments which is highly advantageous for practical application. It is expected that this adsorbent material can be applied for removing arsenic compound from aqueous environment at a lower cost applicable to individual sites serving households or small rural communities, small-scale water treatment system as well as in the developing countries.

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## One-step Fabrication of Nanowire-Grid Polarizers Using Direct Printing Method

황재권, 박경선, 성명모

한양대 화학과

Ag nanowire-grid polarizers(NWGPs)were prepared by a one-step fabrication method,liquid-bridge-mediated nanotransfer molding (LB-nTM). LB-nTM is a new direct nano-patterning methodbased on the direct transfer of various materials from a mold to a substrate via liquid layer. We fabricated NWGPswith Ag nanowire arrays(81 nm parallel lines and 119 nm spaces)on 2.5" transparent substrates by LB-nTMusing an Ag nanoparticle solution.The maximum and minimum transmittancesof the Ag NWGP at 800 nm were 80 % and 10 %, respectively.

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## **Synthesis of Porous Carbon through Electrodeposition of Polypyrrole on Mesoporous Silica Thin Films**

박근영, 장지훈, 권영욱

성균관대 화학과

We report the synthesis of carbon replicas with a nanorod like structure arising from the electrodeposition of polypyrrole into the pores of the mesoporous silica thin films. The mesoporous silica thin film has wormlike and cubic structures. The thickness ranges from 100 to 200 nm and both have pore sizes of 9 nm and wall thicknesses of 4 nm. Polypyrrole was electrochemically synthesized in the pores of mesoporous silica thin films followed by calcination in an inert atmosphere to lead to carbon replica. Factors such as the pore structure of mesoporous silica thin films, counter-anions and calcination conditions are presented in this work. X-ray diffraction(XRD), transmission electron microscopy(TEM), scanning electron microscopy(SEM), ultraviolet-visible spectroscopy(UV-vis) and confocal raman spectroscopy were used for structural analysis. Fourier transform Infrared spectroscopy(FT-IR) and energy-dispersive X-ray spectroscopy(EDS) were used for elemental analysis.

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## **Carbon-supported Pt-Pd-Co tri-metallic nanoparticles as electrocatalysts synthesized via sonochemistry for the oxygen reduction reaction.**

**Matin Md Abdul, 장지훈, 권영욱**

성균관대 화학과

Carbon-supported Pt-Pd-Co tri-metallic nanoparticle electrocatalysts with different atomic ratios were prepared by a facile modified polyol reduction method by ultrasound irradiation. Various characterization techniques such as X-ray Diffraction Analysis (XRD), Scanning Electron Microscopy-Energy Dispersive X-ray Analysis (SEM-EDX), Transmission Electron Microscopy (TEM) and Cyclic Voltammetry (CV) were thoroughly used to determine the average particle size, composition, surface morphology and electrocatalytic properties of the synthesized catalysts. The electrochemical activity of Pt-Pd-Co tri-metallic electrocatalysts was investigated in an electrolyte of 0.1 M HClO<sub>4</sub> saturated by pure O<sub>2</sub>-purging at a room temperature. Oxygen reduction reaction (ORR) on the Pt-Pd-Co tri-metallic system, Pt<sub>1</sub>Pd<sub>0.25</sub>Co<sub>0.5</sub>catalyst showed higher catalytic activity than that of commercial Pt/C catalyst. The electrochemically analyzed results indicate that tri-metallic system can be a promising cathode catalyst for Proton-Exchange Membrane Fuel Cells. This synthesizing method is very simple and has a potential for mass-producing trimetallic system with noble and non-noble metals as electrocatalysts.



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## Electrocatalytic Behavior of Carbon Supported PtFe<sub>x</sub> (x= 0.25~1) Nanoparticles Synthesized by Sonochemistry

장지훈, 권영욱

성균관대 화학과

We report on the preparation of carbon supported PtFe<sub>x</sub> (x= 0.25~1) nanoparticles (NPs) with electrocatalytic activity for fuel cell applications. In order to synthesize the NPs, sonochemical syntheses method was used. Ultrasound irradiation into carbon support, Pt(acac)<sub>2</sub> and Fe(acac)<sub>3</sub> dispersed polyol solution could generate a reducing condition of the precursors which resulted in the formation of bimetallic NPs on carbon support. The structures of the nanoparticles were characterized by XRD, XPS, IR, SEM-EDS, HRTEM and STEM-HAADF. The NPs show narrow size distribution with averaging size of about 2 nm and no macroscopic phase segregation. Electrocatalytic oxygen reduction reaction (ORR) behavior of the materials was measured by rotating disk electrode (RDE) technique and compared with commercial Pt/C (TKK, 37.7 wt%). As a result, we obtained a larger mass and specific activity for ORR on PtFe<sub>x</sub> NPs than commercial Pt/C.

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## Synthesis of gold and mesoporous tungsten oxide nanocomposites

김경재, \*장지훈, \*권영욱

성균관대 물리화학융합과정 \*성균관대 화학과

Ordered mesoporous silica KIT-6 (bicontinuous 3-D cubic, Ia3d) was used as a template to synthesize mesoporous tungsten oxide due to its high surface area, controllable pore size and highly connected open porous networks. Mesoporous tungsten oxide has been reported to be an effective catalyst in the oxidation reaction because of their stability at low pH and has also been used as a support for noble metals. Therefore, the replication of the pores could be a means to produce very good catalyst. In this study, Au/WO<sub>3-x</sub> was synthesized by using infiltration of precursors into the pores of KIT-6 as a hard template and thermal reduction. After heat treatment, silica template was removed by using a HF (10 wt%)/H<sub>2</sub>O/EtOH solution. The synthesized KIT-6 was characterized by Small-angle X-ray scattering (SAXS) and N<sub>2</sub> adsorption-desorption isotherms. The structure of Au/WO<sub>3-x</sub>@KIT-6 and Au/WO<sub>3-x</sub> nanocomposites were confirmed by X-ray powder diffraction (XRPD), Scanning Electron Microscope (SEM) and Transmission Electron Microscope (TEM).

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## High Performance Conducting Polymer-Metal Oxide Hybrid Superlattice Thin Films for Electronic Devices

윤관혁, \*정희찬, 성명모

한양대 화학과 \*한양대 자연과학/화학과

We report a layer-by-layer growth of two-dimensional (2-D) polydiacetylene thin films with inorganic crosslinkers. Additionally, we fabricate organic-inorganic hybrid superlattice structure for flexible electronic devices. In the general molecular layer deposition process, 2-D polydiacetylene films were grown by repeated sequential adsorption of diethylzinc and 2,4-hexadiyne-1,6-diol with Ultraviolet polymerization. Polydiacetylene layers were combined with inorganic zinc oxide crosslinkers, leading to 2-D polydiacetylenes. The hybrid superlattice thin films demonstrated high field effect mobility of  $>23 \text{ cm}^2/\text{V s}$ .

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## Enhancement of Electrocatalytic Activity of Gold NPs for Hydrogen Oxidation Reaction by being Tungsten Oxide-modified carbon support

이은직, \*장지훈, \*권영욱

성균관대 나노과학기술협동학부 \*성균관대 화학과

Previously, we reported that Au NPs could be catalytically active for hydrogen oxidation reaction by sonochemical heating and quenching. However, we also found that the surfaces of the Au NPs are poisoned by the generated protons. In order to further improve the catalytic protonated of the Au NPs, we employed tungsten oxide prepared as a part of the support, by which hydrogen spill-over could be achieved. In this study, two compositions of activated Au NPs supported on WO<sub>3</sub>/C were synthesized by two steps. The first step, amorphous tungsten oxide was prepared by ultrasound irradiation of a solution phosphotungstic acid and a carbon support dispersed in distilled water under Air atmosphere at room temperature. Then, this amorphous powder was heat treated at 550 °C under air to form tetragonal WO<sub>3</sub> on carbon support. The second step, Au/WO<sub>3</sub>/C nanocomposites were prepared by stirring of a solution containing Au NPs and tetragonal WO<sub>3</sub>/C for 24 h. Then, the Au NPs were activated by dispersing Au/WO<sub>3</sub>/C in distilled water and irradiated by ultrasound for 30 min. The obtained nanocomposites were named as Au/WO<sub>3</sub>/C(s)-1, Au/WO<sub>3</sub>/C(s)-2 according to the mass ratio of Au : W = 3 : 1, 1 : 2 respectively. The samples were characterized by powder X-ray diffraction (XRD), energy dispersive X-ray spectroscopy (EDS), and transmission electron microscopy (TEM). Electrocatalytic activity of the samples for hydrogen oxidation reaction was investigated by the linear sweep voltammetry with rotating disk electrode technique (RDE), which showed that the presence of WO<sub>3</sub> enhanced and maintained the catalytic activity of Au NPs.

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발표종류: 포스터, 발표일시: 목 10:30~12:30

## Synthesis of Mesoporous Silica Thin Films with Various Pore Diameters

홍정은, 이기림, 권영욱

성균관대 화학과

We report the synthesis of mesoporous silica thin films (MSTFs) with various pore diameters by using three different kinds of surfactants, Brij-58, F-68, and F-127. The surfactants have different chain lengths, which determine the pore diameters of the mesoporous materials. The pore diameters of the MSTFs synthesized by Brij-58, F-68, and F-127 were 2-3 nm, 5-6 nm, and 9-10 nm, respectively. The MSTFs were characterized by low angle X-ray diffraction (XRD) and transmission electron microscopy (TEM). Platinum nanostructured films were fabricated using the MSTFs as templates by an electrodeposition method. The diameters of the platinum nanorods correspond with the diameters of the template pores. The platinum nanostructured films were probed by scanning electron microscopy (SEM). The surface enhanced Raman scattering effects (SERS) of these platinum films were studied on Rhodamine 6G. The SERS intensities are related with the lengths and the diameters of platinum nanostructure in spite of the same amount of platinum.

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발표분야: 재료화학

발표종류: 포스터, 발표일시: 목 10:30~12:30

## Gas sorption properties of nanoporous COF hybrid materials

허성, 구자민

한국외국어대 화학과

We intend to prepare thermally stable and insoluble in common solvents low density amorphous or crystalline covalent-organic frameworks (COFs) through the click chemistry which forms 1,2,3-triazole ring from azide and polyacetylene. Particularly, to develop efficient hydrogen and carbon dioxide capturing materials, we will prepare 2D or 3D COFs with high surface areas by using azide and polyacetylene compounds with different symmetry. Also the corresponding carbonized derivatives were investigated for nitrogen, hydrogen, and carbon dioxide sorption application.

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## Click Gram-Scale Aqueous Synthesis of Uniform Metal (Cd, Cu, Zn) Hydroxide and Their transformations

고성욱

연세대 금속공학과

Metal hydroxide as sacrificial template is an important material, which is easily transferred into other functional materials, such as metal chalcogenide compounds or metal oxides. This study investigated the large scale synthesis of metal (Cd, Cu, Zn) hydroxide that had controllable and uniform morphology with simple process. The morphology of metal hydroxides can be controlled by simply pouring saturated precursor solutions into pure water, quenching the pH for the metal hydroxides to be precipitated. Under optimized reaction conditions, we could synthesize as much as 2.56 g  $\text{Cd}(\text{OH})_2$  nanowires using 700 ml of cadmium nitrate saturated solution and 1.56 g  $\text{Cu}(\text{OH})_2$  nanobundles using 200 ml of copper nitrate saturated solution. Other merits are that the whole process is carried out by aqueous solution at room temperature within 30s. Since the production scale of process is enlarged, we expect the approach may find immediate industrial applications.

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## **Phenoxazine derivatives with heterocyclic five-membered bridge unit for efficient sensitizers in dye-sensitized solar cells**

이우성, 김재필

서울대 재료공학부

A series of organic chromophores have been synthesized as sensitizers for application in dye-sensitized solar cells(DSSCs). New organic sensitizers have a phenoxazine derivative as an electric donor, five-membered ring as a bridge unit and a cyanoacrylic acid moiety as an electric acceptor as well as an anchoring group. The synthesized dyes were identified by NMR and the photovoltaic properties of the cells fabricated with the dyes were investigated by UV-vis spectroscopy, PL spectroscopy, cyclic voltametry and solar simulator. Among the prepared dyes, a phenoxazine dye containing furan moiety showed improvement of photovoltaic performance ( $\eta=4.35\%$ ) compared to phenoxazine dyes with thiophene moiety and with no additional bridge unit. This was attributed to an increase of short circuit current caused by extended light absorptions of the dye through the introduction of furan moiety.



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## **One step fabrication of organic single crystal nanowires by using liquid-bridge-mediated nanotransfer molding for field effect transistor**

오현석, 양다솜, 성명모

한양대 화학과

In recent years, conductive-conjugated molecules have fascinated scientists all over the world because of their electronic and physical properties. These nanostructured organic single crystals have received great attention because of their potential application in semiconductors, sensors, electronic display, solar cell, and etc. We report a one step fabrication of organic single crystal nanowires that made on Si substrates by liquid-bridge-mediated nanotransfer molding (LB-nTM) with polyurethane acrylate (PUA) mold. LB-nTM is based on the direct transfer of various materials from a mold to a substrate via a liquid bridge between them. In liquid bridge-transfer process, the liquid layer serves as an adhesion layer to provide good conformal contact and form covalent bonding between the organic single crystal nanowire and the Si substrate. The patterned Organic single crystal nanowires and micro structure have been investigated by Transmission Electron Microscopy (TEM), X-Ray Diffraction (XRD), Scanning Electron Microscopy (SEM) and electrical properties.

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발표종류: 포스터, 발표일시: 목 10:30~12:30

## Synthesis and characterization of novel coronene chromophores

최준, 이우성, 김재필

서울대 재료공학부

Two novel coronene compounds were successfully synthesized through a simple one-step reaction in mild conditions with considerable yield. These chromophores are highly stable and much hypsochromic compared to Perylene-3,4:9,10-tetracarboxdiimide and exhibit strong, bright emission. Their stability and high strength yellow color can be especially valuable since in general the high stability and  $\epsilon$  of the yellow chromophores are hard to be achieved. They can be used as good yellow chromophores or fluorophores for a wide range of applications, such as energy relaying dyes of DSSC or yellow compensating dyes for LCD color filter, according to their characteristic range of absorption and emission peaks.

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발표종류: 포스터, 발표일시: 목 10:30~12:30

## Alignment control of Liquid Crystal Molecules using sub 20nm Indium Tin oxide Pattern

정현수, 전환진, 김정현, 손백식, 정희태

KAIST 생명화학공학과

We describe a new molecule alignment technique using second sputtering lithography that enables fabrication of ultrahigh-resolution (ca< 15nm) and high aspect ratio (ca. 10) patterns of indium tin oxide (ITO). We found that the patterned ITO simultaneously acts as an electrode and nano-groove for the alignment of liquid crystal (LC) molecules over large area without any alignment layers. This method not only avoids the high-temperature process, dust and ion contamination caused by previous methods employing polymers for alignment layers, but also provides systematic studies of anchoring energy in terms of height and period of ITO pattern that allow us to investigate critical dimensions of pattern for the alignment of LCs. Good electro-optical responses from liquid crystal light modulators that are formed in this manner suggest utility for fundamental studies and potential practical future application such as flexible display.

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## **The effect of the position and shape of additional methoxy groups introduced to triphenylamine donor on the efficiency of dye-sensitized solar cells**

**김세훈, \*최준, \*김재필**

서울대 공과대 재료공학부 \*서울대 재료공학부

New organic sensitizers containing additional methoxy groups on triphenylamine donor were synthesized for dye-sensitized solar cells (DSSCs). The dyes had a triphenylamine moiety as an electron donor, methoxy groups as additional donors, furan as a  $\pi$ -spacer and a cyanoacrylic acid group as electron acceptor. The structures of the synthesized dyes were analyzed by  $^1\text{H}$  NMR and GC-MS. The optical and electrochemical properties of these dyes were obtained by spectrophotometer, spectrofluorometer and cyclic voltammetry. The photovoltaic cells were fabricated with these dyes and their efficiencies were measured under simulated AM 1.5 irradiation condition. Electrochemical impedance spectroscopy analysis was performed to investigate the interface charge transfer process occurring among the  $\text{TiO}_2$ /dye/electrolyte system in the cell. The highest solar energy-to-electricity conversion efficiency was achieved with a dye which had a 1,4-dioxane structure as an additional donor.

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## Synthesis of bay-substituted perylene diimide dyes for black matrix of liquid crystal display

육심별, 이우성, 김재필

서울대 재료공학부

Organic dyes has recently been suggested to replace carbon black-black matrix. We synthesized bay substituted perylene-3,4,9,10- tetracarboxylic diimide dyes. To enhance thermal and light stability of the dyes, aryl substituents were linked to the perylene at 1 or 1, 7 bay positions by C-N coupling. Structures of the dyes were identified by NMR, mass spectrometry and elemental analysis. The optical and thermal properties of the dyes were measured through UV-spectrometry, TGA and DSC. Dye-based black matrices were fabricated with the synthesized dyes. Thermal stability of the black matrices were measured and their chromatic values were recorded on a color spectrophotometer. The synthesized dyes, especially mono-substituted ones, showed high photophysical properties suitable for black matrix.

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## **In vitro toxicity of aluminum coated colloidal silica nanoparticles**

석지현, 이상복

KAIST 나노과학기술대학원

The alumina-coated, colloidal silica nanoparticles have been widely used for the isolation of plasma membrane and the identification of membrane proteins. The characterization of membrane proteins is important for understanding the mechanism of the cancer cells and developing new cancer drug, since more than 50% of the commercially available drugs target membrane proteins. However, silica nanoparticles are doubted to be endocytosed into the cell and influence on the metabolism and the viability of cells, because the concentration of silica nanoparticles used for the isolation of plasma membrane proteins is pretty high. The endocytosed silica nanoparticles throughout the cell organelles, including the vesicle, cytoplasm, and nuclear membrane were observed with the transmission electron microscopy (TEM) images. Moreover, the cytotoxicity of silica nanoparticles was identified with the WST-1 and LDH (lactate dehydrogenase) toxicity assay method for the both MCF-7 breast cancer cell and NIH 3T3 fibroblast cell lines. In addition, the toxicity of the bare colloidal silica nanoparticle was also studied and the contribution of alumina coating toward the toxicity was characterized.

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## The Mechanism of Corrosion and Pre-passivation of Fe in Borate Buffer Solution

김현철, 김연규

한국의국어대 화학과

Borate 완충용액에서 Fe 의 양극산화반응 mechanism 을 연구하였다. Fe 표면에  $\text{OH}^-$ 이온의 흡착은 Langmuir adsorption isotherm 에 따르는 강한 화학 흡착으로 보였으며,  $\text{OH}^-$ 이온의 흡착 후 산화반응에 의해 Fe 표면의 pre-passivation 현상이 관측되었다. Pre-passivation 에 의하여 생성되는  $\text{Fe}(\text{OH})_2$ 는 탈수반응에 의하여 FeO 로 변화한다. 그러므로 Fe 의 pre-passive film 은  $\text{Fe}(\text{OH})_2$ 와 FeO 로 구성된 것으로 보인다.

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## Optimization of flexible energy-saving electrochromic devices based on Prussian blue analogues

정영희, 박준영, 김영일

부경대 화학과

Recently we have developed wet-coating method for Prussian Blue(PB) film electrode on a conducting plastic substrate such as PET/ITO. In this method solvent-dispersive PB nanopowder was utilized with silica sol. The resulting PB film was transparent and robust and it showed very long-term stability for redox cycling. Prussian blue analogues(PBAs) such as Cu-PBA, Co-PBA and Ni-PBA have the same structure and similar electrochromic properties as Prussian blue(PB). However, solvent-dispersive PBAs are hard to be prepared. In this study, we prepared solvent-dispersive PBA nanoparticles by controlling the reaction temperature, mixing rate and molar ratio of reactants, Utilizing these solvent-dispersive PBA nanoparticles the PBA films on flexible conductiong substrates such as PET/ITO and OEN/ITO were fabricated by wet coating method of silica-sol. The redox and electrochromic properties of these PBA electrodes were comparatively investigated. The flexible electrochromic film devices were assembled by the combination of the PB and PBA electrodes with a polymer-gel electrolyte. PB/Ni-PBA, PB/Cu-PBA, PB/Co-PBA devices(ITO/PEN, 25cm<sup>2</sup>) showed electrochromic color change between blue and bright color, these response times were 9s to 15s. EC devices were maintained high contrast ratio during 1,500 cycles and more.



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## The effect of Carbon coated $\text{Li}_4\text{Ti}_5\text{O}_{12}$ using chitosan for the Lithium ion secondary Batteries

한현주, 정옥상, \*도칠훈, \*\*진종성, \*\*정의덕

부산대 화학과 \*한국전기연구원 전기재료연구본부 전지연구센터 \*\*한국기초과학지원연구원  
하이테크부품소재연구지원센터

The  $\text{Li}_4\text{Ti}_5\text{O}_{12}$  powders were synthesized by using the sol-gel method with Lithium acetate, Titanium isopropoxide and chitosan as a carbon precursor material for an anode of a lithium-ion battery. The pure  $\text{Li}_4\text{Ti}_5\text{O}_{12}$  powders was calcined at 400°C for 6 hours and then calcined at various temperatures (650°C, 750°C and 850°C) in air atmospheres for 2 hours respectively. The chitosan added  $\text{Li}_4\text{Ti}_5\text{O}_{12}$  powders was prepared by added to chitosan using the pure  $\text{Li}_4\text{Ti}_5\text{O}_{12}$  powders. And then the materials were calcined at temperatures 500°C in Ar/H<sub>2</sub> atmospheres for 2 hours. We characterized the synthesized compounds via the crystallinity, confirm of carbon, atom image mapping and their shapes using TGA, XRD, SEM-EDX, TEM, XPS and Nano SIMS. We found that the synthesized powders were carbon-coated using Nano-SIMS and TEM images. We observed voltage characteristics and initial charge-discharge characteristics according to the C rate in  $\text{Li}_4\text{Ti}_5\text{O}_{12}$  electrodes. The obtained initial specific capacity of the chitosan added  $\text{Li}_4\text{Ti}_5\text{O}_{12}$  powder was 113mAh/g with excellent cycle stability which is much larger than that 89mAh/g of pure  $\text{Li}_4\text{Ti}_5\text{O}_{12}$  powder at 0.2C rate.

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## Synthesis and Characterization of $\text{Li}_4\text{M}_{0.15}\text{Ti}_{4.85}\text{O}_{12}$ (M=Cu, Al, Sn, V) anode materials for Lithium ion Batteries

한현주, 정옥상, \*도칠훈, \*\*진종성, \*\*정의덕

부산대 화학과 \*한국전기연구원 전기재료연구본부 전지연구센터 \*\*한국기초과학지원연구원  
하이테크부품소재연구지원센터

Attempts to dope Cu, Al, Sn and V are made for  $\text{Li}_4\text{Ti}_5\text{O}_{12}$ . The effects of dopant on the analysis of physical and electrochemical properties of  $\text{Li}_4\text{Ti}_5\text{O}_{12}$  were investigated. Compared with the undoped  $\text{Li}_4\text{Ti}_5\text{O}_{12}$ , doped  $\text{Li}_4\text{M}_{0.15}\text{Ti}_{4.85}\text{O}_{12}$  have improved structure stability and enhanced lithium ion diffusivity brought about by metal ion doping. The materials were characterized by using XRD, TGA, SEM, XPS. We observed voltage characteristics and initial charge-discharge characteristics according to the C rate in  $\text{Li}_4\text{Ti}_5\text{O}_{12}$  and  $\text{Li}_4\text{M}_{0.15}\text{Ti}_{4.85}\text{O}_{12}$  electrodes. We experiments AC impedance spectroscopy for these synthesized materials. The  $\text{Li}_4\text{Ti}_5\text{O}_{12}$  compound shows a relatively a good discharge capacity of 164 mAh/g at a rate 0.2 C. Compared with the undoped  $\text{Li}_4\text{Ti}_5\text{O}_{12}$ , the metal ion containing  $\text{Li}_4\text{M}_{0.15}\text{Ti}_{4.85}\text{O}_{12}$  samples have high discharge capacities.

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## Synthesis of functionalized silicon nanoparticles and influence of Ru(II) dye adsorption properties on the conversion efficiency of DSSCs

박규학, 김강진

고려대 화학과

Highly efficient dye-sensitized solar cells (DSSCs) through enhancing the short-circuit photocurrent density by incorporating functionalized Si nanoparticles (Nps) into the  $\text{TiO}_2$  film of the DSSCs have been developed. The incorporation of functionalized Si Nps into the  $\text{TiO}_2$  film is expected to extend the light absorption spectral region more toward longer wavelengths than that achieved by widely used Ru(II)-bipyridine dyes. The extension of the light absorption range will lead to an enhanced short-circuit photocurrent density. The feasibility of using silanization as a general tool to functionalize the surface of silicon Nps has been investigated in detail. Silicon Nps were prepared from reduction of silicon tetrachloride with sodium naphthalide. The terminal chloride on the surface of as synthesized particles was substituted by methanol followed by water. The Nps were then silanized by 2-(carbomethoxy)ethyltrichlorosilane. These treatments yielded allylamine termini on the Nps surfaces. The NPs were characterized by TEM, NMR, FTIR and UV-Visible spectra. Changes of terminal groups brought various functionalities to the NPs without loss of the photophysics of the original Nps.

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## Low bandgap polymers in dye-sensitized solar cells

황윤화, \*표명호

순천대 인쇄전자공학과 \*순천대 화학과

1991 년의 Grätzel 팀에 의해 개발된 이래로, 나노 결정의 다공성  $\text{TiO}_2$  를 기반으로 한 높은 에너지 변환효율과 낮은 제조 비용을 갖는 염료감응형 태양전지(Dye-Sensitized Solar Cells)에 대한 연구가 광범위하게 되어왔다. DSSCs 를 구성하는 중요요소에는 photoanode, counter electrode, 그리고 redox couples 을 포함하는 electrolyte 가 있다. DSSCs 의 작동원리는  $\text{TiO}_2$  에 흡착된 dye 가 조사된 빛을 흡수하여 들뜬 상태가 되고 여기된 전자는  $\text{TiO}_2$  의 conduction band 로 주입된다. 이 전자는 나노 결정 구조의 다공성  $\text{TiO}_2$  를 통해 TCO 로 이동한 다음 외부회로를 따라 counter electrode 로 전달되는 과정을 통해 전류를 생성한다. Oxidized dye (cations)는  $\text{I}^-$  redox mediator로부터 전자를 받아 바닥상태로 regeneration 되고, cations 과  $\text{I}^-$  간의 산화환원 반응에 의하여 생성된  $\text{I}_3^-$ 는 counter electrode 표면에서 다시  $\text{I}^-$ 로 환원된다. DSSCs 의 효율에는 여러 가지 요소들이 영향을 미칠 수 있는데, 가장 중요한 결정요인 중 하나가 dye 의 효과적인 regeneration 이다. 이를 위하여 counter electrode 에서의 에너지 손실을 줄이기 위하여  $\text{I}_3^- + 2\text{e}^- \rightarrow 3\text{I}^-$  반응 시 낮은 과전압과 높은 전기전도도를 가지고 전기화학적 환원반응의 촉매적 활성이 뛰어난 소재를 필요로 한다. 일반적으로 위와 이유로 Pt 가 sputtering 또는 thermal decomposition 등에 의해 TCO 에 coating 된 전극이 많이 사용된다. 그러나 Pt electrode 는 장시간 요오드 전해액에 접촉하는 경우 소량의 백금이 산화-용출되어 요오드와 착제( $\text{PtI}_4$  또는  $\text{H}_2\text{PtCl}_6$ )를 이룰 뿐 아니라, photoanode 로 부터 탈착된 dye 가 Pt 표면에 흡착되어 redox couple 의 산화환원 반응을 방해한다고 알려져 있다. 게다가 Pt 는 고가라는 단점을 가지고 있다. 본 연구에서는 NIR 을 흡수하는 polymer 를 photoanode 또는 counter electrode 로 사용하여 효과적인 광변환 및  $\text{I}^-$  regeneration 이 일어나도록 시도하였다.

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## Electrochemical sensors based on functionalized redox active gold nanoparticles

곽규주, \*S. Senthil Kumar, 이동일

연세대 화학과 \*Department of Chemistry Yonsei University

The development of modified electrodes with improved stability, sensitivity and selectivity is the focus of recent research efforts in the field of electroanalytical chemistry. We present the synthesis of highly stable quantum sized Au<sub>25</sub> monolayer-protected gold clusters (MPCs) and their use in electrochemical sensors based on their excellent electrocatalytic activities. To prepare the Au<sub>25</sub>MPCs modified electrode on a glassy carbon electrode, the Au<sub>25</sub>MPCs were entrapped into the sol-gel network formed by the hydrolysis, condensation and polymerization of ethyltrimethoxy silane precursor. The cyclic voltammogram of the modified electrode exhibited well-defined and reversible redox peaks with a formal potential at 0.34 V vs Ag/AgCl corresponding to Au<sub>25</sub>MPCs<sup>0/1-</sup> couple. The modified electrode exhibited dramatic enhancement in the anodic peak current upon the addition of ascorbic acid, demonstrating the electrocatalytic activity. To improve the selectivity, the ligand shell of the Au<sub>25</sub>MPCs was functionalized using ligand exchange reactions. In addition, the electron transfer dynamics in the modified electrode was investigated as a function of Au<sub>25</sub>MPCs, which manifests the dual role of Au<sub>25</sub>MPCs as an electronic conductor as well as a redox mediator.

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## Electrochemical Deposition of Ultrathin Palladium Overlayers on Gold Nanocrystals and Their Application to Direct Formic Acid Fuel Cells

김병권, 송현준, 곽주현

KAIST 화학과

Nanocrystals receive great attention from many researchers for several decades because of their unique properties. In particular, researches in the field of synthesis of bimetallic nanocrystals showed outstanding results for the past five years. In this research, Au/Pt bimetallic nanocrystals were synthesized by electrochemical deposition method. Well-defined Au nanocrystals (octahedron and cube) were synthesized by solution based reduction. Electrochemical deposition conditions for Pd overlayers on Au nanocrystals surface were carefully regulated by controlling parameters of cyclic voltammetry. Surface area and mass of the deposited Pd overlayers were measured by electrochemical methods. In case of less negative deposition potential, the amounts of deposited Pd mass and surface area were small. However, the formic acid catalytic activity of the Pd overlayers was increased even though the Pd surface area and mass were low. We believe that this kind of unprecedented result derived from edge effect and electron inducing effect by Au nanocrystals.

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## Synthesis of Hydrophobic Ionic Liquids for Ion-Sensing at a micro-Liquid/Liquid Interface

김세빈, 장혜리, 이혜진

경북대 화학과

In this poster, we present a simple method to synthesize a hydrophobic ionic liquid (IL) and its applications as an alternative to an organic phase with an organic supporting electrolyte at ITIES (interface between two immiscible electrolyte solutions). As an example, a hydrophobic ionic liquid is synthesized simply by mixing the both of solutions, tetrahexylammonium bromide (THA+Br-) and lithium tetrakis(pentafluorophenyl)borate etherate (TB-Li+) prepared in a mixture of water and acetone. Electrochemical properties of the newly formed ionic liquid, THA+ TB-, working as both an organic supporting electrolyte and an organic phase for micro-ITIES was thoroughly characterized using cyclic voltammetry. In particular, the transfer reaction of various ionic species including tetramethylammonium ion and proton across a micro-interface between water and ionic liquid (micro-L/IL) is investigated. The assisted transfer behavior of proton across a micro-L/IL by the proton selective ionophore, present in the ionic liquid, is also characterized.

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## GLUTATHIONE PROTECTED Au<sub>25</sub> CLUSTERS FOR THE SELECTIVE DETERMINATION OF ASCORBIC ACID AND DOPAMINE

**S. Senthil Kumar**, \*곽규주, \*이동일

*Department of Chemistry, Yonsei University* \*연세대 화학과

Huge amount of electrochemical research has been devoted to the development of chemically modified electrodes (CMEs), as researchers attempt to exert more control over the chemical nature of an electrode. The search for novel materials to design sensitive, selective and stable electrochemical sensors is of great significance at present. Though many methodologies are applied for improving the selectivity of the sensors, the widely used strategy is to introduce charged species during the modification process. Thiolate protected gold nanoparticles have received considerable attention recently because of their unique size-dependent electrochemical, optical and catalytic properties and also the thiolate ligands can be engineered for any specific applications. In the present work, we have studied the electrochemical behaviour of glutathione protected Au<sub>25</sub> clusters (Au<sub>25</sub>GSH) for the first time and utilized them for the selective determination of biologically significant analytes namely ascorbic acid (AA) and dopamine (DA). Au<sub>25</sub>GSH has been synthesized using the modified Brust-Schiffrin method. The synthesized particle had shown absorbances at around 320, 395, 436 and 665 nm, characteristic of Au<sub>25</sub>GSH. Au<sub>25</sub>GSH modified electrode (AuGSHME) has been fabricated by entrapping gold nanoparticles into a sol-gel network and immobilizing on the electrode surface. The cyclic voltammogram of the modified electrode exhibited well-defined redox peaks with a formal potential of 0.24 V in 0.1 M KCl at a scan rate of 20 mVs<sup>-1</sup>. Under neutral pH, the modified electrode has shown excellent catalytic activity towards the electrochemical oxidation of AA and DA, nearly at the same potential. The catalytic currents were found to vary linearly with the concentration of the analyte added, based on which calibration graphs have been obtained. At the modified electrode, the oxidation potentials of these two analytes were found to shift based on the pH of the supporting electrolyte, which is attributed to the change in the charge of the



Au<sub>25</sub>GSH at different pH conditions. Under optimum pH, these two analytes have been determined without the interference of each other.



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## Preparation of Sn/Natural graphite by Sn reduction from tin oxalate

서효리, 이종원, \*이철우, 김 건

고려대 화학과 \*성신여대 화학과

We have been studied the synthesis of a Sn-based natural graphite (Sn/NG) composite as an anode material of lithium ion secondary batteries by Sn reduction on the surface of the spherical natural graphite, and the reduced Sn particles was compared according to the different synthesis time and temperatures. Tin oxalate ( $\text{SnC}_2\text{O}_4$ ) was used as Tin(II) precursor and reduced by sintering at various temperature, 400 – 900 °C under  $\text{H}_2$  atmosphere for 10 hours. The obtained powder was characterized by X-ray diffraction (XRD), field emission-scanning electron microscopy with energy dispersive spectroscopy (EDS) and Fourier transform infrared spectroscopy (FT-IR) to verify Sn reduction. We checked the existence of the reduced spherical Sn particles, and the particle size became small and showed as having a pretty even distribution. The electrochemical properties and their charge/discharge behavior was evaluated using coin cells consisting of the Sn/NG, lithium metal anode, 1M  $\text{LiPF}_6$  in EC/EMC/DMC (3:3:4 v/v) electrolyte and separator (polypropylene). Then, the constant current and controlled voltage (CC-CV) mode electrochemical charge and discharge tests were performed between 0.01 – 1.5 V versus  $\text{Li/Li}^+$  with 0.2 C-rate.

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## Staircase Cyclic Voltammetry (SCV) - Fourier Transform Electrochemical Impedance Spectroscopy Studies on Zinc Oxidation in Dilute Alkaline Solutions

고영훈, \*박수문

울산과학기술대 친환경에너지공학부 \*울산과학기술대 에너지공학부

Electrochemical behaviors of zinc in alkaline solutions are becoming increasingly important primarily because zinc is employed in electrochemical generators as an anode. The zinc-air cell shows good cell performance as it has high energy and power densities due to its large cell voltage thanks to the large negative reduction potential of zinc and its favorable oxidation kinetics. To study the electrode kinetics of zinc oxidation, we conducted staircase cyclic voltammetry (SCV)-Fourier transform electrochemical impedance spectroscopy (FTEIS) combined experiments. The SCV-FTEIS experiment is unique in that it allows a complete kinetic analysis to be made by obtaining impedance data for an electrochemical reaction in real time while the potential is varied [1]. Whereas the conventional FRA method employs the frequency scanning through the whole frequency range, SCV-FTEIS method uses a small potential step signal to acquire impedance data in a wide frequency region throughout the whole voltage range scanned. With the SCV-FTEIS experiments, we report the electrode kinetics for zinc oxidation in alkaline solutions under a variety of experimental conditions. By analyzing raw impedance data thus obtained we report circuit parameters of the electrode/ electrolyte interface for zinc oxidation including capacitances ( $C_d$ ), solution resistances ( $R_s$ ), polarization resistances ( $R_p$ ), and Warburg impedances ( $W$ ) as a function of potential scanned. We then report electrode kinetic information such as the exchange rate constant( $k^0$ ) and transfer coefficient ( $\alpha$ ), the corrosion potential ( $E_{\text{corr}}$ ), the half-wave potential ( $E_{1/2}$ ), and the mass transport characteristics on zinc oxidation in dilute alkaline solutions by analyzing the circuit parameters obtained from impedance data.

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발표종류: 포스터, 발표일시: 금 10:30~12:30

## Synthesis of Si/Natural graphite for a LIB anode material

이종원, 서효리, \*이철우, 김 건

고려대 화학과 \*성신여대 화학과

Silicon is attractive material as an anode of lithium ion secondary batteries for its high capacity, theoretically about 4000 mAh/g, following  $4.4\text{Li} + \text{Si} \leftrightarrow \text{Li}_{4.4}\text{Si}$ . Therefore, partial addition of the silicon into the other anode materials for composite electrodes can improve the cell capacities very well. We have tried to make Si/Natural graphite (Si/NG) composite materials through synthesized Si loading on the surface of the spherical natural graphite by Si reduction. However, there exist the formed particle distribution and its purity, yet. Its electrochemical properties and their charge/discharge behavior was evaluated using the prepared coin cells consisting of lithium metal anode, 1M  $\text{LiPF}_6$  in EC/EMC/DMC (3:3:4 v/v) electrolyte and separator (polypropylene). Then, the constant current and controlled voltage (CC-CV) mode electrochemical charge and discharge tests were performed between 0.01 – 1.5 V versus  $\text{Li/Li}^+$  with 0.2 C-rate except for the initial cycle with 0.05 C-rate.

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## **Amperometric Strip-sensors utilizing Micro-ITIES for Parathion and Methyl Parathion Quantification**

**Md. Mokarrom Hossain, Mengesha Thrusew Tegafaw, 이혜진**

경북대 화학과

In this presentation, we demonstrate an amperometric strip-sensor based on the selective proton transfer reaction across a micro-interface between two immiscible electrolyte solutions (micro-ITIES) for parathion and methyl parathion molecules. Both analytes are dissociated by the hydrolytic reaction with the organophosphorus hydrolase (OPH) in the aqueous phase followed by generating two protons and para-nitrophenol. The generated proton is then transferred across a microelliptic interface between the water and polyvinylchloride-2-nitrophenyloctylether (PVC-NPOE) gel via the assistance of a proton selective ionophore, ETH1778 present in the gel layer. The amperometric signal associated with the assisted transfer of protons is characterized by cyclic voltammetry and differential pulse stripping voltammetry. All electrochemical measurements are performed using our newly developed proton selective strip-sensor fabricated with a polydimethylsiloxane (PDMS) molding on a plastic template and screen printed Ag/AgCl electrodes.

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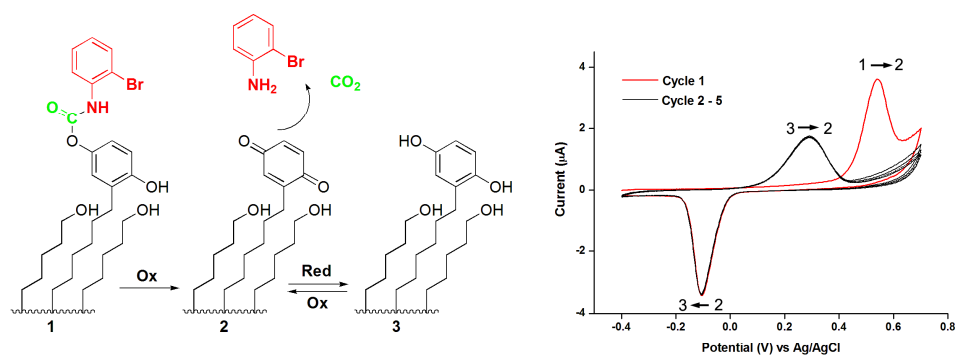
발표종류: 포스터, 발표일시: 금 10:30~12:30

## Programmed Release of Amine-Containing Molecules Based on Electroactive Self-Assembled Monolayers

홍대화, 강경태, 홍석표, 최인성

KAIST 화학과

In this work, we developed self-assembled monolayers (SAMs) of alkanethiols on gold that can release amine groups, when an electrical potential was applied to the gold. The strategy was based on the introduction of the electroactive carbamate group, which underwent the two-electron oxidation with simultaneous release of the amine molecules, to alkanethiols. The synthesis of the designed thiol compounds was achieved by coupling isocyanate-containing compound with hydroquinone. The electroactive thiols were mixed with hydroxyl-containing alkanethiol [HS(CH<sub>2</sub>)<sub>11</sub>-OH] to form mixed monolayers, and cyclic voltammetry was used for the characterization of the release. The mixed SAMs showed a first oxidation peak at +540 mV (versus Ag/AgCl reference electrode), demonstrating irreversible conversion from carbamate to hydroquinone with simultaneous release of the amine groups. The second and third cycles showed typical reversible redox reaction of hydroquinone and quinone: the oxidation and reduction occurred at +290 mV and -110 mV, respectively. This new SAM-based electrochemistry would be applicable for direct release of biologically active molecules that contain amine groups.



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## **Determination of NADH oxidation with MWCNTs-Pd nanoparticles and poly (3, 4-ethylenedioxyrrole) modified electrode.**

유정민, 전승원

전남대 화학과

We have developed and characterized the performance of a NADH biosensor based on MWCNTs-Pd nanoparticles and poly(3,4-ethylenedioxyrrole). The PEDOP/MWCNT-pd/GCE was easily prepared in a rapid and simple procedure, and its application is improved the sensitive of NADH determination. Meanwhile, the results obtained from each cyclic voltammetry (CV) and amperometric methods for NADH determination were comparable. Based on the result of the amperometric method, the response time was very short, and the line of regression equation was obtained even at the very low concentration region of less than 1.0 mM. The proposed NADH biosensor exhibited a wide linear range from 1  $\mu$ M to 13 mM and a low detection limit of 0.18 $\mu$ M (S/N=3), over applied potential of 0.42V by amperometric method. The resulted sensor shows fast response and good stability.



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## **A hydroxylamine electrochemical sensor by multi-walled carbon nanotubes-Pd modified glassy carbon electrode**

이은희, 전승원

전남대 화학과

Hydroxylamine is known as a kind of reducing agent and is widely used for industrial and pharmaceutical applications. It is identified as a key intermediate in the nitrogen cycles and production of nitrous oxide. Determination of hydroxylamine is very important for biological process studies and industrial purposes. Electroanalytical techniques were proven to be relatively direct and effective for the detection of hydroxylamine. We are presenting a sensor for hydroxylamine based on multi-walled carbon nanotubes-Pd modified glassy carbon electrode. The MWCNT-Pd modified GCE exhibited catalytic activity toward the electro-oxidation of hydroxylamine. The results show that there is a dramatic enhancement of the anodic peak current of hydroxylamine oxidation with a linear response ranging, resulting in highly sensitive, fast-response, and good stability sensors.

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## **PEDOP/MWCNT–Pd nanoparticles characterized for Simultaneous determination of dopamine and serotonin in the presence of ascorbic acid**

김슬기, 전승원

전남대 화학과

A chemically modified electrode based on the poly 3,4-ethylenedioxy pyrrole (PEDOP)–coated multi-walled carbon nanotubes (MWCNT) - palladium nanoparticles (Pd) based glassy carbon electrode (GCE) was described for the simultaneous determination of dopamine (DA) and serotonin (5-HT). Electrochemical determination of DA and 5-HT has been studied at modified GCE in 0.1 M phosphate buffer solution (PBS) using cyclic voltammetry (CV) and differential pulse voltammetry (DPV) at pH 7.4 over interfering biomolecule ascorbic acid (AA). The GCE was modified by Pd functionalized MWCNT with electrochemical deposition of PEDOP which investigated by SEM and EIS gradually. This biosensor was best in response compared to other modified electrodes that made in the same lab. Furthermore, the wide linear range, low detection limit and good reproducibility were determined for DA and 5-HT, respectively; and peaks were found 0.165mV and 0.35mV for DA and 5-HT respectively.

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## Electrocatalytic O<sub>2</sub> reduction to water at MWCNT-Pt modified electrode in acidic media

MohammadShamsuddin, 김대근, 정해상, 전승원

전남대 화학과

Cathodic dioxygen (O<sub>2</sub>) reduction was performed at a modified glassy carbon electrode (GCE) by multi-walled carbon nanotubes (MWCNT) and platinum (Pt) nanoparticles incorporated and employed as doping agents. Both the electrochemical behavior of MWCNT-Pd nanoparticle matrix and the electrocatalytic reduction of O<sub>2</sub> were investigated using transmission electron microscopy (TEM), cyclic voltammetry (CV) and rotating ring-disk electrode (RRDE) techniques in 0.1 M H<sub>2</sub>SO<sub>4</sub> aqueous solutions. The electrocatalytic reduction of O<sub>2</sub> at the MWCNT-Pt composite film established a pathway of four-electron transfer reductions into H<sub>2</sub>O. Hydrodynamic voltammetry revealed that the modified electrode was catalyzed effectively by the four-electron transferred reduction of dioxygen into H<sub>2</sub>O with minimal generation of H<sub>2</sub>O<sub>2</sub>. The MWCNT-Pt composite film showed a highly efficient electrocatalytic performance. MWCNT-Pt was an effective mediator for the reduction of dioxygen and was responsible for the enhanced catalytic activity.

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## Electrochemical detection of Sudan1 at Nafion/MWCNTs-SH modified Glassy Carbon Electrode

Orogzodmaa Naranchim, 전승원

전남대 화학과

In this study, an electrochemical sensor glassy carbon electrode (GCE) modified with thiolated multiwall carbon nanotube particles and nafion (Nafion/MWCNTs-SH/GCE) for the convenient and sensitive determination of Sudan1 (S1) was prepared by casting Nafion on MWCNTs-SH/GCE surface and compared with GCE, MWCNTs-SH/GCE, MWCNTs-Pd/GCE, and with the same nanotube electrodes also modified with PEDOP. A well defined oxidation peak (+0.58V) were obtained by cyclic voltammetry (CV) and differential pulse voltammetry (DPV) in phosphate buffer solution (PBS) containing MeOH with an accumulation time. The result showed a linear relationship between the S1 oxidation current and concentration of 0.1 $\mu$ M-3 $\mu$ M with a correlation coefficient of 0.993. Limit of Detection was 0.05 $\mu$ M.

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## **Multi-walled carbon nanotubes supported platinum nanoparticles electrocatalysts for oxygen reduction.**

김대근, MohammadShamsuddin, 전승원

전남대 화학과

This paper reports the experimental characterization of multi-walled carbon nanotubes (MWCNT) supported platinum nanoparticles (Pt) catalysts synthesized using a chemical method. MWCNT-Pt catalysts was characterized using electrochemical techniques such as cyclic voltammetry (CV), as well as rotating ring disk electrode (RRDE) to quantitatively obtain the oxygen reduction reaction (ORR) kinetic constants and the reaction mechanisms. The MWCNT-Pt/GCE electrode showed significantly improved ORR activity as well as different ORR mechanisms, to understand the synthesis, X-ray photoelectron spectroscopy (XPS) was used to detect surface structure changes. The XPS results showed that the attachment of Pt onto MWCNT surface was successful and electrochemical impedance spectroscopy (EIS) suggested that the MWCNT-Pt modified GCE was highly conductive and resistance showed very low as 150Ω. MWCNT-Pt catalyst assigned to sites catalytically active towards the ORR, resulting in activity enhancement as well as a mechanism of a four-electron dominant reduction process.

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## Effect of Activation Reagent Ratio on Capacitive Behaviors of Poly(vinylidene fluoride)-derived Activated Carbon Electrodes

김지일, \*박수진

인하대 물리화학부/화학과 \*인하대 화학과

In this study, we prepared the activated carbon processed by chemical activation with NaOH/poly(vinylidene fluoride) (PVDF)-derived carbon ratios in a range of 1:1–4:1. In order to investigate the effect on their capacitive behaviors and the pore structure changes, PVDF-derived carbons were produced by different defects. The x-ray photoelectron spectroscopy was confirmed to test the surface functional groups of the PVDF-derived carbons after activation. The textural properties of the activated carbons were characterized by  $N_2/77\text{ K}$  adsorption isotherms by Brunauer-Emmett-Teller (BET) equation and Barret-Joyner-Halenda (BJH) method. The capacitive behaviors of the activated carbons were investigated by cyclic voltammograms and galvanostatic charge-discharge performance. The pore size of the activated carbon was distributed mainly in small mesopore of 2–4 nm, which was suitable for non-aqueous supercapacitors after activation process. Consequently, the specific capacitance of the activated carbon were improved with increasing fraction of NaOH reagent, indicating that the pore size of the activated MWNT played a key role in the capacitive behaviors.

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## Synthesis and Characterization of Nitrogen-containing Carbon Shells Based on Pyrolysis of Polyaniline Nanospheres for Supercapacitors

김지일, \*박수진

인하대 물리화학부/화학과 \*인하대 화학과

In this study, the nitrogen-containing carbon shells (NCS) were synthesized by pyrolysis from polyaniline nanospheres at various temperatures. The morphologies and surface properties of the NCS were characterized by transmission electron microscopy (TEM) and x-ray photoelectron spectroscopy (XPS) measurements, respectively. The textural properties were investigated by  $N_2/77$  K adsorption isotherms in order to confirm the specific surface area and the total pore volume. The electrochemical performance was analyzed by cyclic voltammograms and charge-discharge profiles to investigate the relationship among the steric structural evolution, the surface functional groups, and the specific capacitances. The prepared NCS were found to gain controllable morphologies and 14–20 nm pore sizes. Moreover, considering the obtained results, the specific capacitance of NCS prepared at 600°C was highest value as high as 122 F/g, resulting from well-developed pore structure as well as improved wettability from the nitrogen functional groups on surfaces.

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## **Influence of Nickel Oxide on Electrochemical Behaviors of Activated Carbons**

장동일, 박수진

인하대 화학과

In this study, the nickel oxide loaded activated carbons (ACs) was prepared by a post-oxidation method including electroless nickel plating at 573 K in air stream in order to enhance specific capacitance and energy density of ACs. The structure and morphology of the prepared nickel oxide loaded ACs were characterized by X-ray diffraction (XRD), and scanning electron microscopy (SEM). The nickel oxide contents on the ACs were verified by x-ray photoelectron spectroscopy (XPS), and the textural properties were analyzed by  $N_2/77$  K isotherms. And, electrochemical properties were characterized by cyclic voltammetry (CV) and galvanostatic charge-discharge tests in 5 M KOH solution. From the results, it was found that the carbon surfaces were significantly coated with the nickel oxide nanoparticles. The nickel oxide loaded activated carbons composite electrodes have good electrochemical performance and high charge-discharge properties. In addition, the prepared samples exhibits a stable cyclic life.



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발표종류: 포스터, 발표일시: 금 10:30~12:30

## Electrochemical Performance of Pt-Ru Nanoparticles Deposited on Binary Carbon Supports for Fuel Cells

김병주

인하대 화학과

In this work, Pt-Ru catalysts deposited on binary carbon supports using mesoporous carbons (MCs) and carbon blacks (CBs) were prepared for fuel cells. The Pt-Ru nanoparticle sizes and morphological structures of the catalysts were analyzed by X-ray diffraction (XRD) and transmission electron microscopy (TEM), respectively. The Pt-Ru loading content was confirmed by the inductive coupled plasma-mass spectrometer (ICP-MS). The electrochemical characteristics were evaluated by cyclic voltammetry with 0.5 M H<sub>2</sub>SO<sub>4</sub> and 1 M CH<sub>3</sub>OH in 0.5 M H<sub>2</sub>SO<sub>4</sub> solution as electrolyte. From the results, the Pt-Ru nanoparticle size and the loading level were found to be dependent on the mixing ratio of two carbon materials. The electrochemical performance of the catalysts was increased with increasing CBs content up to the CBs 30%. Consequently, the Pt-Ru nanoparticles deposited on the binary supports exhibited better performance than the single support, and the best performance was obtained when the mass ratio of MCs and CBs was 7 : 3.

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## Effect of Nitrogen-containing of Mesoporous Carbons on Electrochemical Activity of Pt-Ru Catalysts for Fuel Cells

김병주

인하대 화학과

In this work, mesoporous carbons (MCs) as a catalyst support in fuel cells were prepared by conventional templating method using SBA-15. And the effect of melamine treatment on carbon supports (M-MCs) was investigated with different melamine amounts, i.e., 0, 1, 3, 4, and 5 g per MCs 1 g. Melamine treatment have been done using melamine suspension dissolved in ethyl alcohol, followed by thermal treatment. The surface and structural properties of the M-MCs supports were characterized by X-ray diffraction (XRD) and elemental analysis (EA). The electrochemical activities of the Pt-Ru catalysts were investigated by cyclic voltammetry measurement. As a result, the electrochemical activities of the M-MCs supports were enhanced by the melamine treatment up to 4 g. Further melamine treatment over 4 g led to the decrease of the electrochemical activity.

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## Electrochemical determination of uric acid on reduced graphene oxide-modified electrodes

Md Mohibul Islam Khan, Al-Monsur Jiaul Haque, 김규원

인천대 화학과

Abstract: Reduced graphene oxide-modified electrodes have been used for determination of uric acid (UA) in the presence of ascorbic acid (AA). The modified electrodes were prepared by electrochemical reduction of graphene oxide (GO) sheets deposited electrostatically on amine-terminated ITO surfaces. The modified electrode showed an excellent electrocatalytical effect on the oxidation of UA, which was investigated in phosphate buffer solution by cyclic voltammetry and differential pulse voltammetry (DPV). The oxidation overpotentials of AA decreased significantly and the oxidation peak currents of UA increase drastically at the modified ITO electrode compared to bare electrode. The proposed method can be used for determination of UA in presence of AA more than two orders of magnitude.

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## Ultrasensitive Electrochemical Immunosensor on Reduced Graphene Oxide- Modified Electrode Surfaces

Al-Monsur Jiaul Haque, 강현주, 김규원

인천대 화학과

We report an ultrasensitive electrochemical immunosensor using reduced graphene oxide (RGO) sheets modified indium-tin-oxide (ITO) electrode surface based on the reduction of enzymatically produced benzoquinone (BQ) in presence of  $H_2O_2$ . Reduced graphene oxide modified electrodes have been prepared by electrochemical reduction of graphene oxide (GO) sheets deposited electrostatically on amine-terminated ITO surfaces. Cyclic voltammetry, atomic force microscopy (AFM), Raman spectroscopy and X-ray photoelectron spectroscopy (XPS) have been employed for the characterization of GO and RGO sheets modified ITO surfaces. The developed electrochemical immunosensor enables us to detect an antigen with a very low detection limit (1 fg/mL), which was based on conventional sandwich-type enzyme-linked immunosorbent assay (ELISA) protocol.

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## **Electrochemical immunosensor for CXC Ligand and CXCR2 receptor interaction using impedance spectroscopy**

정새로미, 김동민, 김유정, 심윤보

부산대 화학과

Chemokine Ligands ,CXCL8 and CXCL5, bind to its cognate receptor CXCR2 to induce inflammatory responses, wound healing, tumorigenesis, and neuronal survival. CXCR2 is the receptor for CXCL5 and CXCL8 involved in angiogenic CXC chemokine-mediated angiogenesis. CXCR2 is promiscuous and binds multiple chemokine ligand with high affinity, including CXCL5, CXCL8. CXC chemokine ligands and receptors have been shown to play important roles in mediating non-small cell lung cancer-associated angiogenesis and organ-specific metastases. Compared with CXCL8, CXCL5 was reported to have a higher degree of correlation with NSCLC-derived angiogenesis. Chemokine ligand binds to the N-terminus of the receptor, leading to a conformational change. This conformational change allows for ligand binding to the activation domain of the receptor. Conducting polymer was polymerized on GCE before immobilizing CXCR2 to fabricate sensor probe. CXCL5 was allowed to react with the sensing probe. The sensor probe was characterized using Cyclic voltammetry, Impedance and QCM. Various parameters such as pH, temperature and Ligand concentration were optimized. Keywords : CXCL5; CXCL8; CXCR2; Conducting polymer; immunosensor

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## Effect of aging on the electrocatalytic activity of gold nanoparticles

조경민, 양해식

부산대 화학과

Highly active electrocatalytic nanomaterials are of importance in the performance of fuel cell, batteries, and electrochemical sensors. Much effort has been devoted to achieving high activities via morphology or composition control and/or via thermal, electrochemical, or chemical treatment. Nevertheless, the dependence of electrocatalytic activities on aging has never been investigated. Here we report slow decrease of electrocatalytic activities of AuNPs upon aging, particularly in two aging conditions: (1) AuNPs are electrochemically deposited onto electrode surface and aged in ambient air (2) AuNPs obtained by reducing Au ions using different reducing agents ( $\text{NaBH}_4$ , citrate, and ascorbate) in aqueous phase are aged at  $4^\circ\text{C}$ , and aged Au NPs are coated on electrode surface for electrochemical measurement. The electrochemical oxidation of  $\text{H}_2\text{O}_2$  and formic acid are employed to measure electrocatalytic activity of AuNPs-coated electrodes.

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## **Sensitive Electrochemical DNA Detection Using Low Nonspecific Binding an Amphiphilic Polymer- and Carbon Nanotube-Modified Electrode**

라지불, \*전상용, 양해식

부산대 화학과 \*광주과학기술원 생명과학과

We report an amphiphilic polymer-, carboxylated multiwalled carbon nanotube (CNT)-, silane polymer-, and streptavidin-modified indium tin oxide (ITO) electrode that allows low nonspecific binding and efficient immobilization of DNA, along with good electrocatalytic activities and low background-current levels. The low nonspecific binding results from the well-covering of the CNT and ITO surface with the amphiphilic polymer and silane polymer, as well as the poly(ethylene glycol) groups of the polymers. The streptavidin for DNA immobilization is covalently attached to the carboxylic acid groups of the amphiphilic polymer and CNT. A low surface coverage of CNT on the ITO electrode provides the good electrocatalytic activities and low background-current levels. The fabricated electrode enables us to achieve a detection limit of 100 pM in DNA detection.

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## **Electrophoretic analysis of phthalates based on a SPCE coated sol-gel solution in a microchip with amperometry**

탁성희, \*윤장희, 심윤보

부산대 화학과 \*한국기초과학지원연구원 부산센터

A  $\mu$ -total analysis device assembling work in-channel preconcentration, separation, and electrochemical detection steps has been developed for phthalate. A micellar electrokinetic chromatography separation technique was coupled with three preconcentration steps of two field-amplified sample stacking(FASS) steps and field-amplified sample injection(FASI) step. An amperometric detection method with a screen print electrode coated sol-gel solution containing mercury chloride was applied to detect preconcentrated and separated species at the end of the channel. The method was examined for the analysis of five phthalate of Dibutyl phthalate(DBP), Bis(2-ethylhexyl) phthalate(DEHP), Dicyclohexyl phthalate(DCHP), Diethyl phthalate(DEP), Benzyl butyl phthalate(BBP). Experimental parameters affecting the analytical performance of the method were assessed and optimized.



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## **An Electrochemical Enzyme Immunochip based on capacitance Measurement for the Detection of IgG**

최지혜, \*장수영, \*\*박덕수, \*\*\*장승철

부산대 분자화학기술협동과정 \*부산대 바이오피지오 센서 연구소 \*\*부산대 바이오피지오 연구  
소 \*\*\*부산대 바이오피지오 센서기술연구소

This poster describes the development of an electrochemical immunochip for the measurement of IgG. Interdigitated immunochip platforms were fabricated by sputtering gold on a glass wafer by using MEMS process and then were coated with Eudragit S100, an enteric polymer, forming an insulating layer over the working area of electrodes. The breakdown of the polymer layer was exemplified by the catalytic action of urease which, in the presence of urea, caused an alkaline pH change. This subsequently caused an increase of the double layer capacitance of the underlying electrode. Used in conjunction with a competitive immunoassay format, this allowed the ratio of initial to final electrode capacitance to be directly linked with the concentration of analyte. The operation mode and the full performance details of the integrated system will be described in the poster.

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## Electron transfer process in the biomimetic layer and superoxide sensor

정진욱, 최영진, \*원미숙, 심윤보

부산대 화학과 \*한국기초과학지원연구원 부산센터

A radical sensing was constructed based on a conducting polymer (poly-5,2':5',2''-terthiophene-3'-carboxylic acid, poly-TTCA) formed on the Au nanoparticles, which were deposited on a screen-printed carbon electrode; the probe was modified with biomaterials including cyt c, lipids (1,2-dioleoyl-sn-glycero-3-phosphoethanolamine (DOPE) and cardiolipin), and ubiquinone, which are involved in electron transfer sequence in the cell membrane. To eliminate affection of foreign biological species, we assembled a lipid bilayer using the LB technique by controlling the density of the outward lipid layer. The optimum experimental conditions for analysis were investigated and a calibration plot for super oxide detection as obtained between  $5.0 \times 10^{-6}$  M and  $1.0 \times 10^{-6}$  M at the optimized condition. The characteristics of the biomimetic layers were investigated by cyclic voltammetry, impedance spectrometry. Keyworld : biomimetic layer, cytochrome c, superoxide, radical

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## Simultaneous separation and sensitive detection of $\beta$ ? Blockers with a microchip using Cyclodextrin modified electrode

Hegde Rajesh, Pranjal Chandra, 심윤보

부산대 화학과

A simple and sensitive on-chip preconcentration, separation, and electrochemical detection for the trace analysis of  $\beta$  ? Blockers has been developed. The method was examined for the analysis of five  $\beta$  ? Blockers. Working electrode was fabricated by covalently immobilizing cyclodextrin onto a gold nanoparticles deposited (3',4'-diamine-2,2';5',2"-terthiophene polymer film at screen printed electrode. The modification of electrode surface has improved detection performance by enhancing signal to noise characteristic without surface fouling of the electrode. Chronoamperometry was used to monitor the redox current at 1.30 V vs. Ag/AgCl. The formation of each layer was confirmed using XPS, SEM, and QCM. The experimental parameters affecting the performance of microchip in terms of amount of immobilized cyclodextrin, temperature, pH, etc were optimized. The detection limit was obtained for all the five  $\beta$  ? Blockers. In future, the developed method will be applied for  $\beta$  ? Blockers detection in real samples. Key words :  $\beta$  ? Blockers Trace analysis; Microchip; Electrochemical detection

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## **An Immunosensor Combined with Aptamer-metal Bioconjugate for Detection of Cancer Marker**

**Ye Zhu, Pranjali Chandra, 심윤보**

부산대 화학과

An immunosensor was developed by covalently immobilizing antibody, which was associated with cancer, onto gold nanoparticle (AuNP) comprised conducting polymer layer, poly-[2, 5-di-(2-thienyl)-1H-pyrrole-1-(p-benzoic acid)] (poly-DPB). The prepared probe was used to react with cancer marker, and then combined with aptamer-metal bioconjugate to form a sandwich type sensing format. The signal was generated and amplified by stripping of the metal label to achieve high sensitivity. The formation of DPB(AuNP) nanocomposite was demonstrated by TEM and UV-visible spectrum. The modification of the immunosensor was characterized using SEM and XPS. The parameters that could affect the sensor response, such as antibody concentration, reaction time, pH, and temperature, were optimized. The calibration plots was constructed and the detection limit was determined. The immunosensor will be used to detect cancer cells for a real sample analysis.

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## Development of Miniaturized Potentiometric Calcium Ion Microsensor

장경, \*심준호, \*\*이영미

이화여대 화학 나노과학과 \*이화여대 신재생에너지연구센터 \*\*이화여대 자연과학대학/화학전

공

Calcium ion ( $\text{Ca}^{2+}$ ) plays important biological/physiological roles particularly in signal transduction such as neurotransmission, muscle contraction, etc. To measure the local  $\text{Ca}^{2+}$  concentration changes in biological samples, we demonstrate the development of a miniaturized  $\text{Ca}^{2+}$  ion selective electrode (ISE) based on micropore. The  $\text{Ca}^{2+}$  ISE is fabricated as follows: (1) A microdisk electrode is prepared by thermal fusing Ag wire ( $r = 75 \mu\text{m}$ ) in a glass capillary; (2) The Ag microdisk is etched to produce a micropore; (3) Ag base surface in the pore electrode is treated with  $\text{Cl}^-$  resulting Ag/AgCl; (5)  $\text{Ca}^{2+}$  ion selective membrane is applied on the pore electrodes for the electrode selectivity to only  $\text{Ca}^{2+}$ . The feasibility of the developed ISE is tested by calibration procedures using a Ag/AgCl reference electrode. The  $\text{Ca}^{2+}$  ISE is expected to be applied to biological research. 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 (2010-0004653).

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## Carbon-Supported Bimetallic AuPd Material as Electrocatalyst

김지영, \*심준호, \*\*이종목, \*\*\*이영미

이화여대 나노화학과 \*이화여대 신재생에너지연구센터 \*\*이화여대 화학과 \*\*\*이화여대 자연과학대학/화학전공

In this presentation, we demonstrate the synthesis and characterization of non-platinum bimetallic AuPd nanoparticles supported on carbon (AuPd/C). By modification of Au, generally known to be a poor electrocatalyst, with Pd, much improved electrocatalysts could be prepared. The prepared AuPd/C catalysts were characterized by transmission electron microscopic (TEM), energy dispersive spectroscopy (EDS), UV-vis spectroscopy to examine the structural features and the ratios of respective metal compositions. The electrocatalytic activity and stability of the AuPd/C for oxygen reduction reaction in acidic media was measured by rotating disk electrode (RDE) polarization experiments. In addition, the methanol tolerance of the AuPd/C was confirmed to find the possible use as cathode catalysts in direct methanol fuel cell (DMFC). This research was carried out under the General R/D Program of the Daegu Gyeongbuk Institute of Science & Technology (DGIST), funded by MEST.

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## Electrocatalytic Activity of Bimetallic AgPt and AgPd in Alkaline Media

양지혜, \*심준호, \*\*이종목, \*\*\*이영미

이화여대 화학나노과학전공 \*이화여대 신재생에너지연구센터 \*\*이화여대 화학과 \*\*\*이화여대  
자연과학대학/화학전공

In general, Ag itself is not a good electrocatalyst. Therefore, the modification of Ag with other metals can provide a great opportunity to improve the catalytic properties. In this presentation, we synthesized supportless AgPt and AgPd bimetallic nanowires, by galvanic replacement reaction using Ag nanowires and corresponding metal precursors. The structures and morphologies of these nanomaterials (i.e. AgPt and AgPd) were characterized by X-ray diffraction (XRD), scanning electron microscopy (SEM) and transmission electron microscopy (TEM). In addition, their electrocatalytic activity for oxygen reduction reaction under alkaline conditions and ethanol tolerance were examined to find the possible use as cathode catalysts in fuel cells. This research was carried out under the General R/D Program of the Daegu Gyeongbuk Institute of Science & Technology (DGIST), funded by MEST.

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## Detection of a Single Nucleotide Polymorphism in IL28B Gene Associated with Chronic Hepatitis C

Pranjal Chandra, Ye Zhu, 심윤보

부산대 화학과

Chronic hepatitis C (CHC) affects > 175 million individuals worldwide and is the lethal liver disease characterized by infection with the hepatitis C virus (HCV). We present a method for the rapid and sensitive detection of a specific SNP in IL28B gene on chromosome 19 which was found in people affected chronic hepatitis C (CHC). A sensor was developed for CHC detection by immobilizing a single-stranded oligonucleotide probe on to the gold nanoparticles deposited 2, 2',5', 2''-terthiophene-3',3''-(p-benzoic acid polymer (pTTBA)) film that was complementary to the IL28B gene segment. The detection was based on changes in the electrochemical response of toluidine blue and impedance spectra of the probe after hybridization with SNP-DNA. A metal ion was further used to discriminate between single mismatch DNA and SNP-DNA using impedance spectroscopy, XPS, and stripping voltammetry. The formation of each layer of sensor probe was confirmed with XPS, and SEM. The experimental parameters affecting the performance of SNP sensor in terms of amount of immobilized DNA, temperature, pH, reaction time etc were optimized. The dynamic range for SNP detection was determined between 0.1 pM and 400 nM with a detection limit of  $5.2 \pm 0.3$  fM (RSD  $\leq 5\%$ ). The present sensor exhibited a long term stability of 2 months.



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## Laser Ablation of Polymer film and Its Application for Electrochemical Sensor

김경태, \*최지혜, \*\*장승철, \*\*\*박덕수

부산대 바이오 센서연구소/분자과학기술 \*부산대 분자화학기술협동과정 \*\*부산대 바이오피지  
오 센서기술연구소 \*\*\*부산대 바이오피지오연구소

In this work, ultraviolet pulsed laser ablation of polyimide film was performed to make nano-sized structures on the polyimide surface to apply electrochemical sensors. Lasers have been used for as effective tools in micromachining including micro patterning and surface modification of several materials. Laser ablations are suitable for those applications of sensor platform that demand more precision, speed, and simple fabrication procedure. The nano structure of polyimide enhances the surface area and effectively increases the sensitivity of sensor devices. The interaction of pulsed ultraviolet laser irradiation with polyimide surface leads to ablative photodecomposition. This technique eliminates the need for photo-masks and allows material patterning directly. After laser ablation of polyimide film, its surface was coated with thin layer of Au or Pt to give a conducting surface. To confirm the electrochemical characteristics of nano structure of polyimide,  $\text{Fe}(\text{CN})_6^{3-}$  was used for standard electro active materials and characterize current and peak potential of  $\text{Fe}(\text{CN})_6^{3-}$ . We also studied the electrochemical sensing ability for analysis of some biological and organic materials with enzyme modified polyimide electrode.

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## New Cathode Redox Polymer in Biofuel Cell

최영봉, 김혁한

단국대 화학과

Biofuel cells have a tremendous opportunity to provide for powering implantable medical devices, leading to less intrusive implantable devices with longer lifetimes. This paper introduce a novel cathode redox polymer based on mediated oxygen reduction by bilirubin oxidase. We report on the four-electron electrocatalytic reduction of  $O_2$  to water under the physiological conditions (pH 7.4, 0.1 M NaCl, 37.5 °C). The new redox polymer formed of poly-N-vinylimidazole by coordinating to  $[Os(ter-py)(dmo-bpy)]^{2+/3+}$  (where ter-py is 2,2':6',2''-terpyridine and dmo-bpy is 4,4'-dimethoxy-2,2'-bipyridine) electrically connected to the reaction center of bilirubin oxidase from *Myrothecium verrucaria* on the screen printed carbon electrodes(SPCEs). We have investigated enzymatic electrocatalytic cascade formulations that have the optimal potential of redox polymer with the enzyme to achieve maxium current densities and longer stability of the electrodes.

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발표분야: 전기화학

발표종류: 포스터, 발표일시: 금 10:30~12:30

## Electricity generation with microbial fuel cells using a polyviologen-modified anode

김준현, 박원철, \*김성현

건국대 생명공학과 \*건국대 특성화학부생명공학과

In a traditional microbial fuel cell (MFC), many kinds of dissolved electron mediators have been used. However, problems associated with those mediators are that electron-transfer rate depends on the diffusion rate of mediator molecules, which put a serious limitation on the performance enhancement as well as their high cost and toxicity to microbes. Although recent studies show that direct electron-transfer is possible via cytochrome and microbial nanowires, power enhancement has not been much achieved. Here we show a different kind of approach for the direct electron-transfer in which a redox mediator acting as a molecular wire connects between microbes and the electrode. We synthesized polyviologen (PV) as a possible molecular wire. PV turned out very effective in accepting electrons from *E. coli* in the presence of substrate. When applied to the electrode surface after mixing PV with carbon black, the cell voltage rose more rapidly than when without PV and the higher power density was resulted, implying that PV properly functioned as a molecular wire.

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## Glucose sensor using a MWCNT-Os composite wire electrode.

전원용, 김혁한, 최영봉, 김남혁

단국대 화학과

In the work, we report on the electrocatalytic oxidation of glucose using the directly electrostatic adduct of Osmium complexes and glucose oxidase on MWCNT electrode. A series of electro-active osmium complexes were prepared and then characterized using the electrochemical techniques. The MWCNT-Os composite wire electrode were prepared by following as: (1) Rinse the MWCNT wire (2) the MWCNT stored in the solution of the synthesised  $[\text{Os}(\text{bpy})_2(4\text{-amp})\text{Cl}]^{+/2+}$  at 4 °C for 24h. The surface morphology of the modified MWCNT-Os composite wire electrode was examined by scanning electron microscopy (SEM). The electrical signals were measured by electrochemical technique. The resulting catalytical oxidation currents were linearly related with the concentrations of glucose.

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## 다중 비가역 흡착으로 변형된 금 전극표면의 백금 덮힘율 연구

김세철, 김영래, \*김잔디, \*이충균

충남대 분석과학기술대학원 \*충남대 화학과

본 연구에서는 다중 비가역 흡착 방법을 이용하여 다결정성 금 전극표면을 변형시키고, 다양한 분석방법을 활용하여 금 전극 표면의 백금 덮힘율에 대한 연구를 하였다. 표면이 잘 연마된 금 전극에 여러 농도의 백금 용액( $10^{-3}$  M~ $10^{-5}$  M)을 사용하여 비가역 흡착 시키고 환원한 후, CO 벗김 전하량, 수소 흡탈착 전하량, 산화백금 환원 전하량, 산화금 환원 전하량 및 광전자분광기와 주사터널링현미경을 사용하여 백금의 덮힘율을 관찰하였다. 연구 결과 비가역 흡착된 백금의 덮힘율 측정에서 수소 흡탈착 전하량을 이용하여 계산한 값이 다른 방법을 사용한 것에 비해서 약 50~60 % 이상 차이가 나타나는 것을 관찰하였다. 즉 일반적으로 백금의 표면적을 측정하는 방법으로 사용하는 수소 흡탈착 전하량 측정은 매우 낮고, 작게 형성된 나노 구조체에서는 정확한 측정 방법이 아님을 알게 되었다.

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## Quinone electrochemistry in aqueous solutions : Effect of proton availability, hydrogen bonding and anions

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건국대 생명공학과 \*건국대 특성화학부생명공학과

We have synthesized quinone molecules that have long alkyl chains of different lengths ( $C_n$ NHC-3-methoxyphenol-ArCOC<sub>6</sub>SH,  $n = 4, 8, 10$ , and  $16$ ) and alkyl spacers with a -SH group. They are not electrochemically active without electrochemical activation, but they undergo demethoxylation through oxidation triggering, forming o-quinone form, which can be converted to hydroquinone form. These molecules were self-assembled on a Au electrode and their electrochemical properties have been studied using cyclic voltammetry. As the chain length increases, a single redox pair begins to split to two redox pairs in which the new pair is very irreversible and grows at the expense of the main redox peak when a full monolayer is formed. This was interpreted in terms of poor proton availability through the long alkyl chain. These interactions occurred from the formation of the two types of hydrogen bondings, i.e., inter and intramolecular hydrogen bondings present between molecules. When a mixed monolayer was formed with a simple alkanethiol whose length is the similar to that of a spacer, two redox pairs become a single pair, indicating a rapid proton access to the quinone group. Even at a full monolayer, two redox pairs become a single pair when the intramolecular hydrogen bonding is blocked by attaching an acetyl group to the amine site in the alkyl chain. We observed that anions also contributed to electrochemical characteristics. Depending on the hydrophobicity of anions, different degree of rigidity of the interface resulted and thus affected electrochemical characteristics. When strong ion-pairing occurs, a resulting 'solid-like' monolayer structure restricts proton accessibility to the quinone moiety, eventually affecting electrochemistry.

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## **Multi-enzyme modified screen printed carbon electrodes coupled with a nanoparticle-and-enzyme-loaded carbon ink for the detection of phenolic compounds.**

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부산대 바이오 센서연구소/분자과학기술 \*부산대 바이오피지오연구소 \*\*부산대 바이오피지오  
센서기술연구소

A new disposable amperometric bi-enzyme electrode for the detection of phenolic compounds has been developed. The electrodes developed uses horseradish peroxidase and tyrosinase modified screen-printed carbon electrodes prepared using a nanoparticle-and-enzyme-loaded carbon ink. Optimization of the experimental parameters has been performed with regard to buffer composition, pH and operating potential. A co-operative reaction involving tyrosinase and HRP occurs at a potential of  $-50\text{mV}$  vs. Ag/AgCl without the requirement for addition of extraneous  $\text{H}_2\text{O}_2$ , thus resulting in a very simple and efficient system. The operation mode and the full performance details of the integrated system will be described in the poster.

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## Nanoporous Au-Pd Electrocatalyst for Oxygen Reduction Reaction

차아름, \*심준호, \*\*이영미, \*\*\*이종목

이화여대 나노화학과 \*이화여대 신재생에너지연구센터 \*\*이화여대 자연과학대학/화학전공 \*\*\*  
이화여대 화학과

Recently, extensive research has been focused on development of non-Pt electrocatalysts for the efficient oxygen reduction reaction (ORR) due to the high cost of Pt, most commonly used cathode catalyst in fuel cells. For this, we synthesized the nanoporous Au-Pd (npAu-Pd) catalysts via a two-step method. The npAu network structure with a few nanometer size grains was synthesized by the galvanic replacement reaction (GRR) involving Co nanoparticles and Au precursor. Then npAu-Pd was prepared via the second GRR between npAu and various concentrations of Pd precursor. The structure and electrocatalytic activities of npAu-Pd catalysts were characterized by TEM, EDS and rotating disk electrode (RDE) voltammetry. This research was carried out under the General R/D Program of the Daegu Gyeongbuk Institute of Science & Technology (DGIST), funded by MEST.



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## Preparation of Iridium Oxide Nanowires and Their Application to Electrochemical Sensor for NADH

강민경, \*이유민, \*\*심준호, \*\*\*이영미, \*\*\*\*이종목, \*\*\*\*\*김명화

이화여대 전기분석화학 \*이화여대 화학나노과학과 \*\*이화여대 신재생에너지연구센터 \*\*\*이화여대 자연과학대학/화학전공 \*\*\*\*이화여대 화학과 \*\*\*\*\*이화여대 화학 나노과학과

We have prepared highly crystalline iridium oxide ( $\text{IrO}_2$ ) needlelike-nanowires by an atmospheric pressure chemical vapor deposition of  $\text{IrO}_2$  powder at the elevated temperature without the use of catalyst. The structures and morphologies of the  $\text{IrO}_2$  nanowires (IrNWs) were characterized using scanning electron microscopy (FE-SEM), high resolution electron microscopy (HRTEM) and Raman spectroscopy. The IrNWs with high density reveal more than 1  $\mu\text{m}$  long and the diameter of each nanowire was  $\sim 100$  nm. The IrNWs were also grown on a Pt wire surface (dia. 25- $\mu\text{m}$ ), IrNW-Pt, which was tested as an amperometric microsensor. The electrochemical properties of the fabricated IrNW-Pt microelectrode were also examined for the redox reactions of  $\text{H}_2\text{O}_2$  and coenzyme NAD(H) mediating assays and transformations of a broad range of biochemicals.

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## Thioether-Bridged Organosilica Based Hollow Carbon Capsule as a Highly Efficient Catalyst Support in Proton Exchange Membrane Fuel Cell

김정호, 김민식, \*Nitin Chaudhari, \*\*chaudhari kiran, \*\*\*양대수, \*송민영, \*김윤경, \*최혁수,  
\*박진솔, \*최은지, 권선영, 유종성

고려대 신소재화학학과 \*고려대 소재화학과 \*\*고려대 소재화학 \*\*\*고려대 신소재화학

The novel synthesis and characterization of hollow carbon capsules from thioether-bridged organosilica (TBOS) is reported. The TBOS-based hollow carbon capsules (HCCs) with uniform macropores of about 200 nm in diameter and 3 ~ 5 nm mesopores in the shell were synthesized by carbonization of organic moiety of TBOS spheres, which were prepared by simple sol-gel reaction of Bis(3-triethoxysilylpropyl) tetrasulfide (TESPTS). Bis(3-triethoxysilylpropyl) tetrasulfide (TESPTS) used as a porogen agent in the synthesis of TBOS contains the organic moiety  $-(\text{CH}_2)_3\text{-S}_4\text{-(CH}_2)_3$ , which can be converted into carbon framework upon carbonization. The HCC possesses fantastic structural characteristics such as high specific surface area, large mesopore volume and well-developed interconnected void structure, which are highly desired for a catalyst support in low temperature fuel cells. The TBOS-based HCCs with hollow macroporous core of ca. 200 nm and ca. 30 nm thick mesoporous shell were explored as an anode catalyst support for proton exchange membrane fuel cell (PEMFC). The HCC-supported 20 wt% Pt<sub>50</sub>Ru<sub>50</sub> has exhibited almost double power density than commercial catalyst support carbon black Vulcan XC-72-supported 20 wt% Pt<sub>50</sub>Ru<sub>50</sub> catalyst, suggesting that the TBOS-based HCC is a highly efficient anode catalyst support in PEMFC.

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## Electrochemical Scanning Tunneling Microscopic Observation of Electrochemical behaviors of Bi modified Pt(111) Electrode Surface

김잔디, \*김세철, 악더라시다, 이충균

충남대 화학과 \*충남대 분석과학기술대학원

본 연구는 cyclic voltammetry 와 electrochemical scanning tunneling microscopy (EC-STM)를 사용하여 개미산 산화에 있어 Pt 전극의 촉매 활성을 증가시키는 외부 금속인 Bi 의 전기화학적 거동을 원자 수준에서 이해하고자 하였다. 0.5 M H<sub>2</sub>SO<sub>4</sub> 에 포화된 Bi 용액에 Pt(111) 전극을 각각 10, 30, 60 초 접촉하여 비가역 흡착을 하였고, 이때 Bi 의 전기화학적 덮힘율은 0.11-0.33 이었고, STM 을 통해 얻은 덮힘율은 0.13-0.33 으로 island, mono-layer, second-layer 의 형태로 흡착하였다. 높은 덮힘율(0.33)의 Bi 가 흡착한 전극의 경우 second-layer 가 형성되는데, 열린회로전압에서 Pt(111) 표면에 형성된 Bi 의 산화층 흡착층의 원자 구조는  $(\sqrt{2} \times \sqrt{2})\text{-BiO}^+$  이었고 전극을 환원시키면 second-layer 가 mono-layer 로 내려앉고, 이때 Bi 의 흡착 구조는  $(\sqrt{3} \times \sqrt{3})\text{R}30^\circ$  으로 덮힘율이 하였다. 그리고 전극의 전압이 환원 전압에서 재 산화 전압으로 변화하여도 비가역적으로 흡착한 Bi 의 원자 구조는 변화하지 않는 비가역적인 거동을 하였다.

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## **A conducting polymer doped with graphene**

박옥경, 송현곤

울산과학기술대 친환경에너지공학부

Redox-active properties of conducting polymers (CPs) have been used for batteries and pseudocapacitance-based supercapacitors. Several drawbacks of CPs could be pointed out when they are used as an active material for electrochemical energy devices. Their electroactivity is kinetically slower than charging or discharging electric double layer. Also, their electric properties changes from conductive to insulating after reduction, losing their charge carrier (e.g. polypyrrole). To overcome those demerits, we incorporated functionalized graphene as a dopant into conducting polymers. It should be noticed that the graphene was used only as a genuine dopant while several prior works prepared composites of conducting polymers with graphene. The electric conductivity of our graphene-doped CPs is superior to its counterpart with a conventional and simple dopant: Even in its reduced state, the graphene-doped CPs still showed fairly good conductivity. Specific capacitance was strikingly enhanced by about 10 times especially at high rate. We believe the material or its modified ones can be used as advanced active materials for high-energy capacitors and high-power rechargeable batteries.

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## 2-step electrodeposition of cadmium selenide on a zinc oxide nanowires modified FTO glass

최승연, 채유진, 이우주, 박지혜, 명노승

건국대 응용화학과

기존에 연구된 CdSe의 electrodeposition은  $Cd^{2+}$  이온과  $Se^{4+}$  이온이 함께 들어있는 전해질을 사용하는 co-deposition이 사용되었다. co-deposition의 경우 CdSe 외에도 Se 및 Cd가 함께 electrodeposition되는 단점을 가지고 있다. 이와 같은 단점을 보완하기 위해 본 연구실에서는 1차적으로 Se를 electrodeposition한 다음  $Cd^{2+}$  이온만 들어있는 전해질에서 일정 전압을 가하여 Se를 Se<sup>2-</sup>로 cathodic stripping 시킴으로써 CdSe를 합성하는 2-step electrodeposition법을 개발한 바 있고 이를 이용하여 CdSe 및 CdTe, ZnSe, ZnTe 등의 합성에 적용한 바가 있다. 본 연구에서는 이 방법을 사용하여 CdSe/ZnO를 합성하였으며 특히 ZnO nanowire에 적용하여 CdSe/ZnO core-shell을 합성하였다. 생성된 CdSe/ZnO electrode는 EDX, XRD, SEM을 통하여 characterization하였다. 또한 생성된 photoelectrode의 흡수특성과 band gap을 계산해 보기 위하여 UV-visible absorbance와 diffuse reflectance를 측정해 보았다. 측정결과 700nm의 파장영역부터 명확한 흡수를 보였고 Kubelka-Munk식을 사용하여 2.2 eV의 band gap을 가진다는 사실을 확인하였다. 마지막으로 생성된 전극의 반도체 성질을 확인하기 위하여 photocurrent를 측정해본 결과 ZnO는 n-type, Se는 p-type, CdSe는 n-type 반도체 성질을 가진다는 사실을 확인하였다. 이러한 실험을 통하여 기대되는 효과는 위에서 설명한 Se와 Cd가 존재하지 않는 순수한 CdSe를 얻을 수가 있고 그외에도 Se layer의 두께를 컨트롤 함으로써 손쉽게 CdSe film의 두께도 조절할 수 있다. 또한 nanowire에 적용한 ZnO/CdSe core-shell의 경우 ZnO nanorod와 CdSe가 heterojunction을 이루고 있으므로 flat한 구조에 비하여 면적에 있어서 큰 장점을 가질 수 있으며 반도체 감응형 태양전지에 응용한다면 전자가 광전극으로 이동하는데 있어 방향성을 가지게 되므로 이동중에 생기는 손실을 확연히 줄일 수 있다.

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## Photoelectrochemical Deposition of CdSe Thin Films on the ZnO-Modified Au Electrode

채유진, 최승언, 이우주, 곽지혜, 명노승

건국대 응용화학과

Photoelectrochemical deposition of CdSe thin films on the ZnO-modified Au electrode using electrochemical quartz crystal microgravimetry(EQCM) and voltammetry is described. First, selenium is deposited on the ZnO modified Au electrode by illumination. And then, Corrosion of pre-deposited Se electrodes by illumination at a fixed potential resulted in  $\text{Se}^{2-}$  species, which was manifest from the EQCM frequency changes.  $\text{Se}^{2-}$  species generated from the photocorrosion reacted with  $\text{Cd}^{2+}$  ions in the electrolyte to form CdSe films on the ZnO modified Au electrode. The deposition of CdSe is confirmed by EDX.

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발표분야: 전기화학

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## Synthesis of Graphene/CNT Composite and Its Electrocatalytic reduction of $\text{H}_2\text{O}_2$

우승희, 정택동, \*박원철, 김하석

서울대 화학부 \*서울대 융합과학기술대학원 나노융합학과

This study demonstrated the effective restraint of the aggregation of graphene sheets by inserting CNTs. We proposed a facile *in situ* chemical procedure to synthesize a graphene/CNT composite material. The composite indicates a homogeneous network with ultrathin graphene nanosheets on nanotube bundles. The cyclic voltammogram of the  $\text{Fe}(\text{CN})_6^{3-/4-}$  redox couple at a graphene/CNT composite modified electrode showed an increased current intensity. In addition, the graphene/CNT composite modified electrode exhibits good electrocatalytic behavior, which is useful for the detection of  $\text{H}_2\text{O}_2$ . In view of the distinguished properties of graphene and CNT, these composites may find promising applications in the fabrication of many devices such as sensors, fuel cells, batteries, and supercapacitors.

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## Surface Modification of Fluorocarbon Thin Films Deposited by Pulsed-Plasma

이지혜, 김강진, \*이연희

고려대 화학과 \*KIST 특성분석센터

The plasma polymerization of fluorocarbon/acetylene mixtures was performed to produce a hydrophobic film on a substrate. Fluorine-containing hydrophobic thin films were obtained by pulsed plasma (PP) and three kinds of fluorine-containing gases such as C<sub>2</sub>F<sub>6</sub>, C<sub>3</sub>F<sub>8</sub>, and c-C<sub>4</sub>F<sub>8</sub> were used. Process parameters for plasma polymerization such as gas ratio, gas pressure, pulse frequency, and processing time were investigated. Especially, we focused on hydrophobicity improvement of film surface as a function of gas ratio. Surface analytical instruments such as TOF-SIMS, XPS, and AFM were used to characterize the fluorocarbon thin films generated by PP. TOF-SIMS was used to provide useful information about the chemical properties including surface composition and XPS was used to examine the chemical structure of the fluorocarbon films. And, film thickness and surface morphology were also observed by using FE-SEM, profiler meter and AFM.



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발표종류: 포스터, 발표일시: 금 10:30~12:30

## Water electrolysis with different sized Co<sub>3</sub>O<sub>4</sub> films prepared by a paste coating method

전효상, \*민병권

과학기술연합대학원대 청정연료 화학공학 \*KIST 청정에너지연구센터

In electrolysis, the obstacle would be an anodic reaction for water oxidation where substantial energy loss occurs mainly due to the large overpotential. Numerous electrocatalysts have been applied to reduce the overpotential in the water oxidation including expensive precious metals (e.g. Ir, Ru, and Rh). In this study, we demonstrate successful fabrication of different sized Co<sub>3</sub>O<sub>4</sub> electrocatalyst films at low temperature ( 50 oC) on a stainless steel substrate by a paste coating method using Nafion as a binder. The structural characteristics of Co<sub>3</sub>O<sub>4</sub> films were investigated by SEM, XRD and BET. We also investigated the electrochemical characteristics of the films with different particle sizes using classical electrochemical analysis. Based on the cyclic voltammetric measurements, the number of active sites of the films was estimated to 57.8, 86.1 and 95.7 mC cm<sup>-2</sup> for the films with particle size of 145.9, 63.3 and 36.5nm, respectively. The highest hydrogen production rate was measured to 39.6 ml/h for the film with particle size of 38.9 nm. The details will be discussed in the presentation.

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## Electrochemical Detection of EGFR Mutations by DNA Hybridization Processes

안영창, 최영봉, 조민호, 윤일규, 김진호, \*장원철, 김혁한

단국대 화학과 \*단국대 첨단과학대학

Mutation in the epidermal growth factor receptor(EGFR) have recently been described in patients with advanced non-small-cell lung cancer(NSCLC). EGFR mutation detection is being offered to aim in clinical decision-making about the use of EGFR tyrosine kinase inhibitors for patients with advanced NSCLC. In this study, a simple electrochemical approach for the detection of EGFR mutations in breast cancer, using gold nanoparticle modified electrodes. This method was used for the discrimination between ssDNA and dsDNA, and the amperometric detection of target nucleic acid fragments. In summary, electrochemical approach is extremely simple, highly sensitive, and specific and has potential usefulness for rapid and reliable detection of EGFR mutations in breast cancer.

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## **Sensitive and simultaneous detection of some anticancer drugs in microfluidic device**

**shabiabbas, Pranjal Chandra, \*원미숙, 심윤보**

부산대 화학과 \*한국기초과학지원연구원 부산센터

This report investigates the simple yet highly sensitive detection of anticancer drugs by integrating the preconcentration steps with a separation step in a microfluidic device using electrochemical detection method. An amperometric detection method with SPCE/AuNPs/pTTBA/CNT/AuNPs/dsDNA was used for the detection of preconcentrated and separated anticancer drugs at the end of separation channel. The preconcentration factor was increased by about 1200 folds as compared with a conventional simple capillary zone electrophoretic analysis using the same channel. The experimental parameter affecting the analytical performances, buffer concentration, water plug length, preconcentration time, and detection potential were examined. This method was also successfully tested for spiked concentrations of anticancer drugs in real human urine. The proposed method has demonstrated for the efficient detection and separation of anticancer drugs in a microfluidic device at extremely low sample concentration.

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## Measurement of nitric oxide in ischemic myocardium via use of a perfluorinated xerogel-derived amperometric gas sensor

김승기, \*이기자, \*박현국, 차근식, 남학현, 신재호

광운대 화학과 \*경희대 의공학교실

Endogenously produced nitric oxide (NO) has been studied extensively in recent years due to its role in numerous physiological processes including vasodilator, angiogenesis, neurotransmission, and phagocytosis. Over the past two decades, several methods have been studied for directly measuring NO including electron paramagnetic resonance spectroscopy, fluorescence, chemiluminescence, and electrochemical sensing. Of these, Electrochemical sensors have several advantages including easy miniaturization, high sensitivity, and simple fabrication. These characteristics are suitable for measurement in vivo for biological systems. However, the electrooxidation of NO requires a relatively high working potential (+0.8 V vs Ag/AgCl); thus, interference from other readily oxidizable biological species precludes selective detection of NO. To improve the selectivity for NO, the electrode surface is modified by xerogel membrane. It is well-known that amorphous, and hydrophobic fluoropolymers are highly permeable to many gaseous species. The use of perfluorinated xerogel-derived gas-permeable membrane is allowed to develop amperometric NO sensors with dramatically reduced interference species, while maintaining high NO permeability. Herein, we demonstrate the utility of the perfluorinated xerogel-modified NO microsensor for measuring the NO levels in vivo. This study provides real-time monitoring of NO in ischemic myocardium utilizing xerogel derived amperometric NO sensor. The concentration changes of NO during ischemia and reperfusion in a rat heart is examined using the sensor. The measurement reflects neuroprotective effect by releasing NO.

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## Study on steel substrate-based dye-sensitized solar cells

이형균, 김강진

고려대 화학과

Several steel products were applied as substrate material for efficient, nanoporous TiO<sub>2</sub> dye-sensitized solar cells (DSSCs) with the aim of improving their the photochemical properties of currently plastic-based flexible DSSCs. Specifically, the metal substrate allows application of high-temperature sintering processes and shows high conductance even after sintering. Among the steel substrates, a DSSC with Zn-coated substrate showed comparable efficiency to the cells with a F-doped tin oxide (FTO) glass substrate under the illumination from the Pt counter electrode (back illumination). Furthermore, the photovoltaic properties were enhanced when the steel substrates were sputter-treated with ITO. A comparison between conventional DSSCs with a FTO glass substrate and DSSCs with steel substrates will be discussed.

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발표종류: 포스터, 발표일시: 금 10:30~12:30

## Studies on fill factor of dye-sensitized solar cells by electrochemical impedance spectroscopy

이강우, 김강진

고려대 화학과

The fill factor(FF) is one of the important parameters of dye-sensitized solar cells(DSSCs) which are related to the cell efficiency. It is defined as the ratio of the maximum power observed in practice to the power limit of the cell in theory. FF is a more sensitive parameter to the experimental condition compared to open-circuit voltage( $V_{oc}$ ) and short-circuitcurrent density( $J_{sc}$ ). FF depends on series resistance( $R_s$ ), charge transfer resistance( $R_{ct}$ ), light intensity and illumination direction. The FF under back illumination was higher than that under front illumination. Based on the electrochemical impedance spectroscopy, the  $R_{ct}$  at the  $\text{TiO}_2$ /electrolyte interface was found to be higher under back illumination compared to that under front illumination. As the light intensity increased, the  $J_{sc}$  and efficiency were increased linearly and the  $V_{oc}$  was saturated. It was interesting to observe that the FF showed a maximum value at 0.75 sun. In this presentation, we report the dependence of FF on electrical elements and light intensity studied by electrochemical impedance spectroscopy.

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발표종류: 포스터, 발표일시: 금 10:30~12:30

## Electrochemical etching behaviors of ITO thin film in sodium nitrate solution

최동철, 손용근

성균관대 화학과

In this study, we focused our attention to the recycle of Indium-tin oxide (ITO) from used Mobile Personal Information Apparatus. The Thin film transistor liquid crystal display (TFT-LCD) is composed of several electrical components i.e. backlight, polarizer, glass, TFT, liquid crystal, ITO, and color filter. We separated TFT-LCD panel into several parts. ITO is one of the most valuable parts for recycling view point. We used electrochemical etching method mainly chronopotentiometry to obtain free glass. We used etching current of 0.1 A and sodium nitrate solution as electrolyte. The composition and microstructure of ITO films were investigated by X-ray photoelectron spectroscopy (XPS), Energy dispersive x-ray spectroscopy (EDS) and X-ray diffraction (XRD). Furthermore, the surface of the films were observed by Field emission scanning electron microscope (FE-SEM), Optical microscope and Atomic force microscope (AFM).

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## Electrochemical desorption of thiolate self-assembled monolayer (SAM) on a gold substrate: Application to the highly sensitive electrochemical copper sensor

이충구, \*이영관, 손용근

성균관대 화학과 \*성균관대 화학공학과

We have studied an electrochemical sensor devices for the detection of copper ion by using thiolate self-assembled monolayer (SAM) formed on a gold substrate. However, the electrochemical desorption of thiolate SAM in liquid environments would seriously limit the appropriate function of thiol-based sensor devices. Thus, when we electrochemically detect the concentration of copper ion, it is important that the electrochemical desorption of thiolate SAM does not occur into the detection potential range. First, we studied the electrochemical desorption of self-assembled 3-mercaptopropionic acid (3-MPA) monolayer on a gold-evaporated wafer. The SAM was formed at the gold substrate surfaces using a 1 mM solution of the modifier in ethanol and tested by cyclic voltammetry and conjugated with FT-IR/ATR. Finally, we electrochemically detected the concentration of copper ion in the potential range, -0.2V to 0.6V vs. an Ag/AgCl (KCl sat'd) electrode. The gold substrate modified with 3-MPA was used for the electrochemical analysis of trace amount of copper ion by square wave anodic stripping voltammetry (SWASV) method. We could identify anodic stripping peak to around 0.3V against Ag/AgCl(KCl sat'd), corresponding to the oxidation of reduced Cu to Cu<sup>2+</sup>.



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## Effects of silicon doped $\text{LiFePO}_4$ as cathode material for Li-ion battery

서가영, 이경은, 신병철, 이영일

울산대 화학과

Lithium iron phosphate ( $\text{LiFePO}_4$ ) has been one of the most promising cathode materials for the second generation of lithium rechargeable battery due to its improved safety, low environmental cost, and high theoretical current capacity (170 mAh/g). However, the poor electronic conductivity of  $\text{LiFePO}_4$  due to the low lithium-ion diffusion rate makes difficulties of its commercial applications. Appropriate element doping could be a potential approach to enhance the electronic conductivity of  $\text{LiFePO}_4$ . Herein, silicon doping in olivine  $\text{LiFePO}_4$  has been applied to improve the electrochemical performances including the rate capability and cycling life. The silicon doped  $\text{LiFePO}_4$  samples have been also characterized by X-ray diffraction (XRD) and scanning electron microscope (SEM).

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## Electrochemical Functionalization of Single-Walled Carbon Nanotube with Amine-terminated dendrimers

이윤선, \*김주훈, 김태현

순천향대 화학과 \*경희대 화학과

Single-Walled Carbon Nanotube (swCNT) was functionalized with amine-terminated polyamidoamine (PAMAM) dendrimers on SiO<sub>2</sub> wafer surface via electrochemical oxidation of the terminal amine groups of dendrimers. The electrochemical functionalization of swCNT with dendrimers was confirmed by cyclic voltammetry (CV) and X-ray photoelectron spectroscopy (XPS). The immobilized dendrimer films were robust and behaved as charge-selective electrochemical gates for oppositely charged redox molecules. The immobilization approach was applied to assemble Au dendrimer-encapsulated nanoparticles (Au DENs, dia.  $1.5 \pm 0.3$  nm) on swCNT/Au/Ti on SiO<sub>2</sub> wafer and the resulting Au DEN films showed electrocatalytic activity to hydrazine oxidation.

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## **An Ultrasensitive Electrochemical Immunosensor for a Cancer Biomarker Based on Multienzyme Mediated Biocatalyzed Precipitation**

악더라시다, \*Md. Aminur Rahman, \*\*이충균

충남대 화학과 \*충남대 분석과학기술대학원 분석과학기술과 \*\*충남대 화학과, 분석과학기술  
대학원 분석과학기술과

Highly sensitive protein detection is critical in clinical diagnostics as it can detect and monitor diseases such as cancer. As a new amplification strategy for protein detections, multiple enzyme label-mediated biocatalyzed precipitation was followed for the development of a highly sensitive electrochemical immunosensor for prostate specific antigen (PSA). Anti-PSA antibody was immobilized on the gold nanoparticles adsorbed thiolated multi-walled carbon nanotube (MWCNT) on a gold electrode. PSA was sandwiched between the Anti-PSA and multiple horseradish peroxidase (HRP)-labeled secondary antibody. Square wave voltammetric (SWV) technique was used to detect PSA through the HRP-mediated biocatalyzed oxidation of 4-chloro-1-naphthol in the presence of hydrogen peroxide. Under the optimized experimental condition, PSA can be detected as low as 1 pg/ml by this method.

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## Electrochemical Chemodosimeter for the Detection of $\text{Cu}^{2+}$ Ion Using Anthraquinone derivatives

김태현, \*김종승, 이유진

순천향대 화학과 \*고려대 화학과

Recently, much attention has been given to the use of chemodosimeters as a chemical sensor through a specific irreversible chemical reaction between dosimetric molecules and target species, leading to a fluorescent/color change in the receptor. Chemodosimeters directed towards the detection and measurement of copper(II) are of particular interest, because  $\text{Cu}^{2+}$  is third in abundance (after  $\text{Fe}^{2+}$  and  $\text{Zn}^{2+}$ ) among the essential heavy metal ions in the human body and it plays a pivotal role in a variety of fundamental physiological processes in organisms ranging from bacteria to mammals.[30–32] Conversely,  $\text{Cu}^{II}$  can be toxic to biological systems when its concentration level exceeds intracellular need and is also capable of displacing other metal ions that act as co-factors in enzyme-catalyzed reactions. However, to the best of our knowledge, no electrochemical chemodosimeter has been reported. Here, we reports the electrochemical chemodosimeter for the determination of  $\text{Cu}^{2+}$  using anthraquinone derivatives via voltammetric methods.

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## 전이금속 산화물을 이용한 전기화학적 리튬 도핑 공정 연구

박민식, 김점수, \*임영근, 김영준

전자부품연구원 차세대전지연구센터 \*고려대 신소재공학과

전기이중층커패시터 (EDLC)의 낮은 에너지밀도를 개선하기 위해 음극 활물질로 리튬 이온을 가역적으로 삽입 / 탈리할 수 있는 탄소계 재료를 이용하는 리튬이온커패시터 (LIC)가 제안되었다. LIC는 이온화 경향이 큰 리튬 이온을 음극에 미리 도핑하여 음극의 전위를 대폭적으로 낮춤을 통해 셀 전압도 종래의 EDLC의 2.5 V 대비 크게 향상된 3.8 V 이상의 고전압 구현이 가능하여 에너지 밀도의 향상을 도모할 수 있다. 이러한 LIC를 구현하기 위해서는 제조 공정 중 음극에 리튬을 사전 도핑하는 안정적인 도핑공정이 반드시 필요하다. 하지만 기존 리튬 도핑방식의 경우 리튬이 음극에 도핑 되는 양을 제어하기가 어렵고 도핑 공정에서 금속 리튬의 안전성을 확보하기 어려운 단점이 있어 양산에 적용하기 위해서는 제조공정의 개선이 필요하다. 따라서, 본 연구에서는 초기 충방전 효율이 낮은 고용량의 전이금속산화물을 양극 첨가제로 적용하여 전기화학적으로 리튬을 음극에 도핑 할 수 있는 새로운 개념의 리튬 도핑방식을 제안하고, 다양한 전이금속 산화물의 양극 첨가제로 적용 가능성을 살펴보고자 한다. 특히,  $\text{Li}_2\text{MoO}_3$ 와  $\text{Li}_5\text{FeO}_4$ 를 이용한 리튬 도핑공정 개발을 위해 전기화학 특성 및 다양한 구조 분석을 통해  $\text{Li}_2\text{MoO}_3$ 와  $\text{Li}_5\text{FeO}_4$ 의 합성 조건을 최적화하고 이를 채용한 리튬 도핑공정이 리튬이온 커패시터의 전기화학적 특성에 미치는 영향에 대해 구체적으로 논의하고자 한다.

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## Demonstrations of ion selective mesoporous silica thin film and polypyrrole deposition into pores

강호석, \*이호춘, \*\*곽주현

KAIST Chemistry \*금오공과대 응용화학과 \*\*KAIST 화학과

A composite electrode was synthesized by mesoporous silica thin film formation on indium tin oxide (ITO) glass electrode. The silica film was prepared from aqueous silica precursor, tetraethoxy orthosilicate (TEOS) sol solution, in presence of cetyltrimethylammonium bromide (CTAB) by silica deposition catalyzed by hydroxyl ion formed by electrochemical potential. In the silica film, the direction of pores are normal to the substrate and ions are permeable through film. The formation of the silica film is tested in various conditions, employing both potentiostatic and galvanostatic methods. The diameter of pores is 4-5nm and the thickness is 100-120nm in the film. After removal of CTAB from the film, ion accessibility to the substrate surface through the pores is demonstrated by cyclic voltammetry (CV) technique using anionic  $\text{Fe}(\text{CN})_6^{3-/4-}$  and  $\text{Ru}(\text{bpy})_3^{2+/3+}$  redox couples as electrochemical probes. Polypyrrole (PPy) was deposited into pores in silica film from pyrrole solution by anodic deposition and the redox reaction of Ppy in the template is measured by means of CV analysis in aqueous solution.

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발표코드: III-ELEC.P-361

발표분야: 전기화학

발표종류: 포스터, 발표일시: 금 10:30~12:30

## Nanoparticles Encapsulated-Dendrimer Monolayer-Based Electrochemical Immunosensor Through Multi-Catalytic Redox Label Amplification

**Md. Aminur Rahman**, \*악더라시다, \*이충균

충남대 분석과학기술대학원 분석과학기술과 \*충남대 화학과

In the present study, we have fabricated a gold nanoparticles encapsulated-dendrimer monolayer based electrochemical immunosensor for a cancer biomarker, carcinoembryonic antigen (CEA). We used catalytic activity of multiple ferrocene labels for the signal amplification of the nanoparticles encapsulated-dendrimer based immunosensor system. Multiple ferrocene labels were conjugated with the secondary antibody via polyethyleneimine/functionalized multi-walled carbon nanotube assembly. The immunosensor probe was characterized using scanning electron microscope (SEM), transmission electron microscope (TEM), x-ray photoelectron spectroscopy (XPS), quartz crystal microbalance (QCM), and electrochemical techniques. The present immunosensor exhibited a wide dynamic range and a low detection limit for CEA.

일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: III-EDEC.P-362

발표분야: 초중등 교사 · 화학교육

발표종류: 포스터, 발표일시: 금 10:30~12:30

## 화학교육을 위한 웹사이트 콘텐츠의 효율적 활용 방안 - 중학교 1

### 학년 화학단원을 중심으로 -

하동수, 이강범, \*박종근

순천대 화학교육과 \*경상대 화학교육과

본 연구에서는 중학교 1 학년 화학교과를 중심으로 교수-학습에 활용할 수 있는 웹사이트를 정리하고 웹 사이트의 콘텐츠를 평가하여 우수한 웹사이트를 선별하였다. 선별된 웹사이트 콘텐츠의 활용 방안을 제시하고 검색엔진(네이버, 다음)을 사용하여 중학교 1 학년 과학교과 2 종(금성출판사, 교학사)의 내용에 충실한 것을 기준으로 선택하여 연구하였다.



일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: **III-EDEC.P-363**

발표분야: 초·중등 교사 · 화학교육

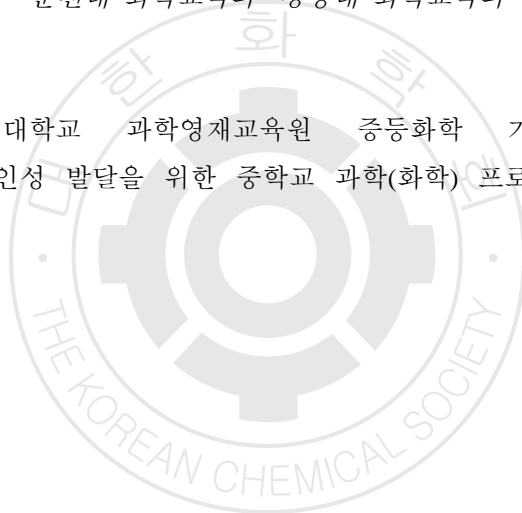
발표종류: 포스터, 발표일시: 금 10:30~12:30

## 창의.인성 발달을 위한 중학교 과학(화학)영재교육 프로그램 교수법

하동수, 이강범, \*박종근

순천대 화학교육과 \*경상대 화학교육과

본 연구에서는 순천대학교 과학영재교육원 중등화학 기초과정 프로그램을 분석하여평가하고 창의.인성 발달을 위한 중학교 과학(화학) 프로그램의 개선점을 제시해보고자 한다.



일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: **III-EDEC.P-364**

발표분야: 초중등교사·화학교육

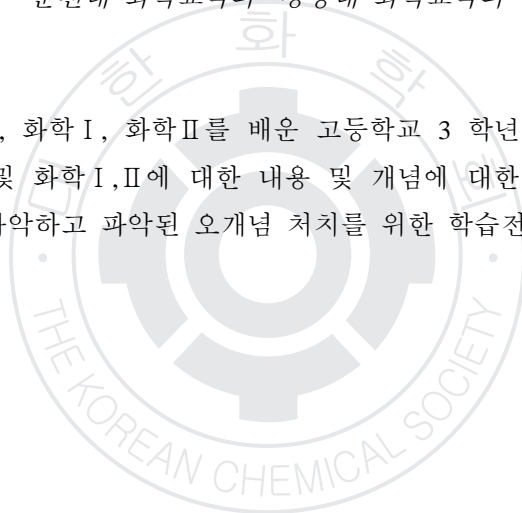
발표종류: 포스터, 발표일시: 금 10:30~12:30

## 고등학교 학생들의 화학의 오개념에 대한 연구

하동수, 이강범, \*박종근

순천대 화학교육과 \*경상대 화학교육과

본 연구에서는 공통과학, 화학 I, 화학 II를 배운 고등학교 3학년 자연계 학생을 대상으로 공통과학 중 화학개념 및 화학 I, II에 대한 내용 및 개념에 대한 이해의 정도와 학생들이 가지고 있는 오개념을 파악하고 파악된 오개념 처치를 위한 학습전략을 제시하고자 한다.



일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: III-EDEC.P-365

발표분야: 초·중·고교사 · 화학교육

발표종류: 포스터, 발표일시: 금 10:30~12:30

## 사범대학 과학교육 전공 예비 교사의 과학 개념 조사와 배경변인에 따른 분석

이현정, 윤혜선, \*최원호

단국대 교육대학원 화학교육 \*한국교육과정평가원 교육평가연구본부

본 연구에서는 사범대학 과학교육과 화학 전공 선택 예정인 예비교사들을 대상으로 국가수준 학업성취도 화학 평가 문항의 이해도를 조사하고 예비 교사들의 배경변인(학년, 고등학교 심화 선택 과목, 대학 심화 전공 또는 선택 예정 심화 전공)에 따른 분석을 실시하였다. 연구 결과 제 7 차 교육과정의 중 3 '혼합물의 분리'단원의 문항, 고 1 '산과 염기', '전해질과 이온' 단원에 해당하는 문항에서 중·고등학교 학생들과 사범대학교 과학교육 전공 1 학년 예비교사들의 정답률이 공통적으로 매우 낮았고, 이는 대학교 1 학년 예비교사들의 대학 입시 수능 과목으로 화학 1, 2 를 선택한 것과 상관없이 대부분의 학생들에게 공통적으로 나타나는 현상이었다. 하지만 화학을 심화 전공으로 선택한 대학교 상위 학년으로 갈수록 해당 문항에 대한 예비교사들의 정답률이 높아졌다. 이 결과의 원인을 찾기 위해 실시한 배경변인에 따른 분석과 심층 면담 연구를 통해 몇 가지 사실을 알 수 있었다. 첫째, 포화 또는 불포화에 따른 용액의 용해도, 물질의 분리 방법, 수용액에서 산의 이온화 과정을 화학 반응식으로 표현하는 것과 전해질의 종류에 따라 다른 전류의 세기에 관한 개념들에 대하여 가진 오개념은 중·고등학교 시절부터 사범대학교 과학교육 전공 1 학년 때까지 잘 변하지 않았다. 둘째, 오개념이 잘 변하지 않는 개념들은 중·고등학교 시절 기본 개념을 이해하기 이전에 계산을 통한 문제 풀이에 익숙해졌거나, 개념은 알고 있지만 실험이나 실생활과 연계된 내용, 그리고 기본 개념을 통해 문제에 제시된 자료(그림, 도표, 등)를 이해하는 특성을 가진 개념들이었다. 셋째, 수능 선택 과목으로 화학 1, 2 를 선택한 것과 상관없이 모두 정답률이 낮았던 이유는 해당 개념에 대한 체계적 이해보다는 기억 위주로 학습을 하였기 때문이다. 넷째, 대학의 화학 심화 전공을 선택함으로써 접하는

여러 실험과 심화 학습 기회를 통해 중·고등학교 시절부터 대학교 1 학년 시절까지 변하지 않았던 과학 오개념을 수정할 수 있었다.



일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: III-EDEC.P-366

발표분야: 초중등교사·화학교육

발표종류: 포스터, 발표일시: 금 10:30~12:30

## 2007년 개정 교육 과정에 의한 중학교 과학 교과서의 비교 분석

### 연구-2학년 교과서를 중심으로.

문숙희, 이상좌

목포대 화학과

본 연구에서는 2010 년도에 중학교에 입학하여 2011 년에 중학교 2 학년인 학생들을 대상으로 사용될 2007 년 개정 교육과정에 의한 중학교 과학 교과서 10 종을 비교 분석하였다. 개정 교육과정에서는 제 7 차 교육과정의 기본 철학을 수용하면서 ‘과학적 소양 함양’ 및 ‘창의성’교육을 강조하였다. 창의성 신장을 위해서 ‘창의성 신장’을 위한 지침, 과학 글쓰기, 토론등이 추가 되었고, 새롭게 도입되는 ‘자유 탐구’에 대하여 제시하였다. 따라서 각 교과서의 구성 체계, 탐구 내용, STS 주제의 읽을 거리, 진로 소개, 과학 글쓰기의 주제 및 교과서의 양적인 면 등에 대하여 상호 비교하여 보았다.

일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: III-EDEC.P-367

발표분야: 초중등교사·화학교육

발표종류: 포스터, 발표일시: 금 10:30~12:30

## 과학영재들의 적용실험 설계 과정에서 나타나는 사고의 특징

유지연, 노태희

서울대 화학교육과

이 연구에서는 중학교 1학년 과학영재 학생들의 적용실험에 대한 실험 설계 과정에서 나타나는 사고를 발생사고법을 이용해 조사하였고, 각 과정 요소별로 과학영재의 수행 정도를 분석하였다. 연구 결과, 과학영재들은 실험을 설계하는 과정에서 ‘상황설정’, ‘전략결정’, ‘가정설정’, ‘측정계획’, ‘가정의 타당화’의 과정 요소와 관련된 사고를 하는 것으로 나타났다. 그러나 이러한 과정 요소에 대한 과학영재들의 수행 정도는 다소 미흡한 측면이 있는 것으로 나타났다. 특히, 실험 설계 과정에서 문제를 해결하는데 적합한 목표 상황을 구체적으로 설정하거나 자신의 사고에 대해 적절한 준거를 통해 비판적으로 점검하는 능력이 부족한 것으로 드러났다. 이에 추상적이고 이해하기 어려운 문제 상황을 학생들에게 친숙한 구체적인 상황으로 바꾸어 생각하도록 하는 새로운 실험 설계 학습 전략의 가능성을 제안하였다. 본 연구의 결과는 실험 설계 능력과 같은 과학적 사고 기술을 강조함으로써 과학적 창의성을 계발하기 위한 과학영재 교육프로그램 개발에 유용한 시사점을 제공할 수 있을 것이다.

일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: III-EDEC.P-368

발표분야: 초중등교사·화학교육

발표종류: 포스터, 발표일시: 금 10:30~12:30

## 학업성취도평가문항의 답지반응에서 발견되는 오답지 반응 분석-

### 2004~2008년 국가수준 학업성취도 화학문항을 중심으로-

신영식, \*최원호

단국대 화학교육대학원 \*한국교육과정평가원 교육평가연구본부

본 연구는 국가수준 학업성취도 평가의 중학교 화학영역에서 반응률이 높은 오답지의 특징을 찾기 위해 중학교 3학년 133명을 대상으로 오답지 선정 이유에 대한 설문을 실시한 연구이다. 본 연구에서는 초등학교 이후 처음 배우는 화학 변화를 다뤄 오개념을 학생들이 많이 가지고 있다고 알려진 '물질의 특성'단원에 속하는 문항을 연구 대상으로 정했다. 선정한 문항은 변별도가 높으며, 반응률이 높은 오답지(10% 이상이거나 정답률과 유사한 반응률)를 가진 문항을 대상으로 하였다. 설문 결과는 오답지를 정답으로 선택한 학생을 중간, 기말고사 성적을 기준으로 3개 그룹(상, 중, 하)으로 나누고, 성적 그룹별로 오답을 선정한 이유를 분석하였다. 이 연구를 통하여 다음과 같은 사실을 알 수 있었다. 첫째, 학생들은 화학반응 단원의 기체 반응의 법칙의 개념을 성취수준별로 다르게 해석하고 있었다. 상 수준의 학생들은 기체 반응의 법칙을 일정 성분비의 법칙과 혼동을 하며 일정한 비의 내용만 숙지하고 문항을 푸는 경향이 나타났다. 중 수준의 학생들은 문항지의 탐구를 통한 문제 풀이가 아닌 법칙의 비만 암기한 상태로 문제를 푸는 경향이 나타났다. 하 수준의 학생들은 문항 접근이 어려워 비를 생각하지 못하고, 문제의 일정한 형태를 보고 정답을 적는 경향이 나타났다. 둘째, 학생들은 화학반응 단원에서 화학식과 입자들의 배열에 관한 개념을 성취수준별로 다르게 해석하고 있었다. 상 수준의 학생들은 화학식과 배열을 비교적 정확히 맞추고 문항을 풀었다. 하지만 CO와 C<sub>2</sub>O<sub>2</sub>의 개념을 약분을 하여서 같은 물질이라고 생각을 하는 경향이 나타났다. 중 수준의 학생들은 입자들의 배열을 통하여 고체, 액체, 기체 등의 문제로 파악한후 비슷한 것끼리 정답을 유추해 나가는 경향이

나타났다. 하 수준의 학생들은 화학식과 입자들의 배열을 매칭을 시키지 못하였고, 화합물과 화학식이 같으면 그것으로 정답을 택하는 경향이 나타났다.





일시: 2011년 4월 28~29일(목~금) 2일간

장소: 제주ICC

발표코드: III-EDEC.P-369

발표분야: 초중등 교사 · 화학교육

발표종류: 포스터, 발표일시: 금 10:30~12:30

## 정보적 텍스트의 유형이 초등 과학 학습에 미치는 효과: 학습자 변 인과의 상호작용 및 효과적인 텍스트의 사회-언어학적 특징 분석

임희준

경인교육대 과학교육과

본 연구에서는 현행 과학 교과서를 중심으로 진행되는 초등 과학 탐구 수업에 보조적 읽기 자료로서 서로 다른 유형의 정보적 텍스트(이야기식 텍스트와 설명식 텍스트)를 제시하고 그 수업의 효과와 특징을 정량적 분석과 질적 분석을 통하여 조사하고자 하였다. 연구 대상은 초등학교 5 학년 3 학급을 대상으로 하으며, 한 학급은 정보적 텍스트를 사용하지 않고 교과서를 중심으로 수업하는 학급으로 비교 집단이다. 정보적 텍스트를 활용하는 실험 집단은 2 학급으로, 각 학급에서는 이야기식 텍스트, 설명적 텍스트 등 서로 다른 유형의 정보적 텍스트를 활용하였다. 연구 대상 단원은 5 학년 ‘기온과 바람’과 ‘물의 여행’ 단원이었다. 연구 결과, 정보적 텍스트를 활용한 실험집단이 비교집단에 비해 학업성취도 총점이 높았으며, 그 중에서도 이야기식 텍스트를 활용한 집단이 설명식 텍스트를 활용한 집단보다 성취도가 높았다. 과학에 대한 흥미에서는 설명식 텍스트를 사용한 집단의 과학에 대한 흥미가 가장 높았으며, 다음으로 이야기식 텍스트를 사용한 집단의 평균이 높았다. 정보적 텍스트를 활용한 수업이 학생들의 과학적 태도에 긍정적인 영향을 미침을 알 수 있었다. 이를 각 유형별 텍스트의 과학적 특성, 문법적 형식, 대인적 기능 등 사회-언어학적 특징을 비교함으로써, 그 이유를 찾아보고자 하였다. 또한 이야기식 텍스트를 활용한 집단과 설명식 텍스트를 활용한 집단이 토론 내용을 비교함으로써 서로 다른 양식의 텍스트를 사용함에 따른 상호작용의 특징을 비교하였다. 동일한 차시에 대한 두 집단의 소집단 토론 과정을 비교한 결과, 조에 따라 토론 내용에 차이가 있기는 하였으나 텍스트 유형에 따른 차이는 별다르게 나타나지 않았다. 단원에 대한 수업을 마친 후, 정보적 텍스트의 활용에 대한 학생들의 인식을 조사하고 비교하였다.

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발표종류: 포스터, 발표일시: 금 15:00~17:00

## **Energy System Analysis of Introducing Energy Amplifier about Energy and Environmental Key Issues**

김희태, 안태규

성균관대 에너지과학과

Energy amplifier is emerging nuclear technology, which can reduce an amount of radioactive waste and its half life to ease waste management burden. But an impact of introducing the technology has not been estimated because its social and environmental impact is complicate to grasp. Social and environmental impacts are being estimated by using life cycle assessment (LCA). It takes into account on not only use phase but also material mining, manufacturing, maintenance, and disposal. Moreover LCA inventories are expanded to include invisible and indirect effects and consequences (consequential LCA). Consequence of introducing energy amplifier can be estimated in energy system view to know comprehensive impact. In this study we analyze environmental and social consequences and energy performance of energy amplifier by using LCA and systemic approach.

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발표종류: 포스터, 발표일시: 금 15:00~17:00

## Soft-template synthesized ordered mesoporous carbon counter electrodes for dye-sensitized solar cells

천진녕

포항공과대 화학공학과

Ordered mesoporous carbon (OMC) with a high surface area ( $\sim 1575 \text{ m}^2/\text{g}$ ) and bimodal pores (2.5 nm and 6.1 nm) was synthesized using a soft-template method employing triblock copolymer F127 as the structure directing agent and then applied as a low temperature processable counter electrode for dye-sensitized solar cells. The OMC counter electrode-based DSSC shows an energy conversion efficiency of 7.46%, whereas that of a Vulcan XC72 counter electrode is 4.30%. Electrochemical impedance spectroscopy analysis reveals decreased charge transfer resistance at the OMC counter electrode-electrolyte interface, thus improved fill factor and energy conversion efficiency.

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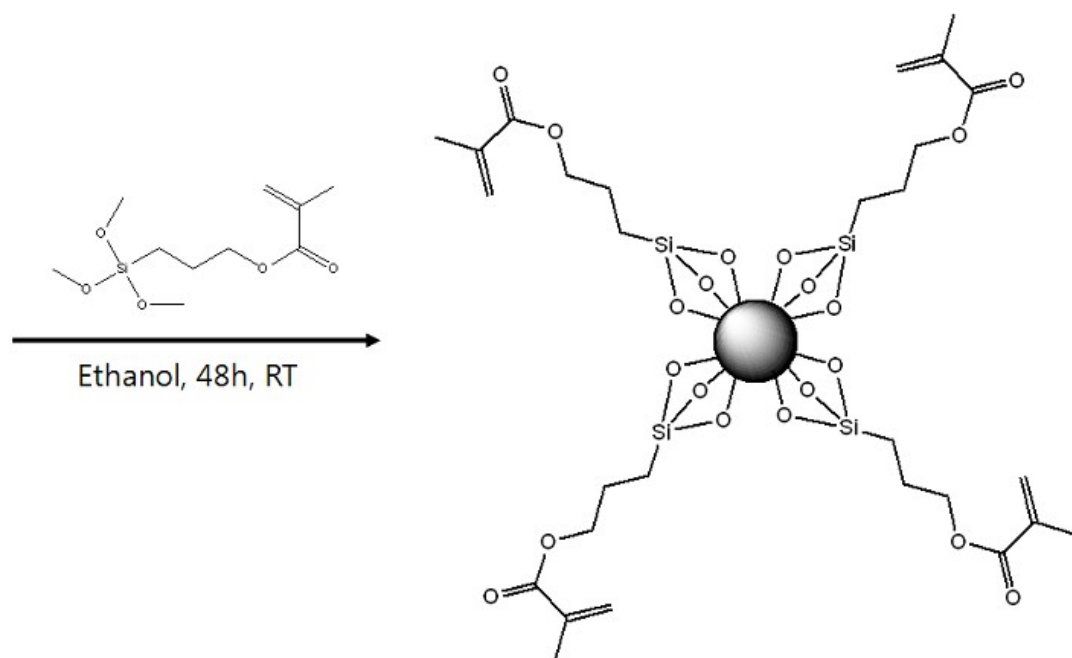
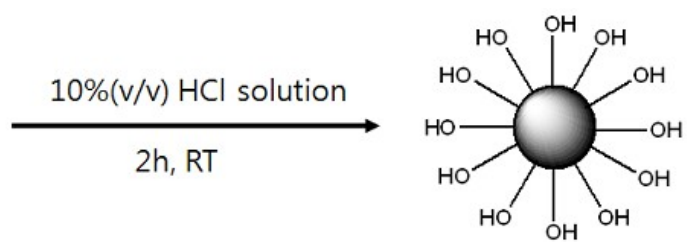
## 염료감응 태양전지용 나노젤 전해질

한치환, \*홍영식

한국에너지기술연구원 태양광연구센터 \*서울교육대 과학교육과

염료감응 태양전지(DSSC)는 광합성원리를 이용한 고효율의 광전기 화학적 태양전지로 1991 년 스위스 EPFL 의 Grätzel 그룹에서 11.1%의 광전변환 효율을 보고하면서 많은 관심을 받았다. 최근에는 일본의 소니에서 두개의 염료를 동시에 사용하여 효율이 9% 이상인 모듈을 개발하여 상용화 가능성이 보다 높은 상황이며, 생산단가를 낮추고 장기안정성을 높이기 위한 연구가 많이 진행되고 있다. 본 연구에서는 효율과 안정성을 동시에 높이기 위해 실리카 표면에 다양한 유기물질을 화학적으로 결합시켜 나노젤 전해질에 적용하였다. 실리카 표면에 유기물질을 도입하기 위해서는 실란커플링 시약을 사용했으며, 매우 단순한 반응에 의해 화학적으로 잘 결합됨을 확인하였다. 합성된 다양한 유기물질이 도입된 실리카 나노물질을 액체전해액과 섞어 젤형전해질을 제조하였으며, 이를 적용한 염료감응 태양전지를 테스트한 결과 유기물질의 종류에 따라 효율이 증가하기도하고 감소하기도함을 확인하였다. 가장 좋은 효율을 나타낸 3-(trimethoxysilyl)propyl methacrylate 이 결합된 실리카 나노젤의 경우 단락전류밀도는  $26.449 \text{ mA/cm}^2$ , 개방전압은  $0.647 \text{ V}$ , 충진율은  $0.456$  으로, 같은 조건에서 액체 전해질의 7.1% 효율 보다 0.7% 높은, 7.8%의 효율을 나타내었다. 이러한 나노젤 전해질의 경우 액체 전해질과는 달리 점도가 높아서 누액의 위험이 없고, 액체 전해질보다 높은 효율을 나타내기 때문에 염료감응 태양전지 상용화 가능성을 높일 수 있을 것으로 판단된다.

  
Silica nano particle



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발표종류: 포스터, 발표일시: 금 15:00~17:00

## Quantitative analysis of Ag nanoparticles using fluorescence dyes for environmental toxicity study

한현숙, 전수지, Ambadas B. Rode, 홍인석, 김상호

공주대 화학과

The environmental toxicity issues of Ag nanoparticles have been a big research theme for scientists as well as researchers in industry. It is believed that the  $\text{Ag}^+$  ions released from the Ag nanoparticles are the toxic material which causes many problems for environment. However, it is still a controversy that whether the nanoparticle itself is also toxic for environment. We have carried out the environmental toxicity study of Ag nanoparticles and  $\text{Ag}^+$  ions released from them separately. The fluorescence spectroscopy of custom designed organic dyes which react with  $\text{Ag}^+$  ions makes it possible to analyze the environmental toxicity issues of Ag nanoparticles and the  $\text{Ag}^+$  ions separately.

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발표종류: 포스터, 발표일시: 금 15:00~17:00

## **The Photovoltaic Performance with Ionic liquid based electrolytes for Dye-sensitized solar cells**

이경주, 이현정

현대하이스코 환경에너지연구팀

The dye-sensitized solar cells (DSCs) provide a promising alternative to conventional p-n junction photovoltaic devices because of their relatively high efficiency, simple fabrication process and low production cost. DSCs using organic liquid electrolytes have received significant attention because of their high power conversion efficiency. However, the important drawback of the DSC using liquid electrolyte is the less long-term stability due to the volatility of the electrolyte contained organic solvent. Several approaches have been used to overcome such problems by replacing of the volatile liquid electrolyte with a solid-state hole conductor, quasi solid-state gel electrolyte or ionic liquid electrolyte (IL). However, the efficiencies of DSCs with these alternative media are usually less than that of DSCs with organic liquid electrolyte, which is attributed to a higher ionic transport resistance of such media compared with that of liquid electrolyte. In this study, we prepared ionic liquid based electrolytes. We analyzed the characteristics of DSC with the different additional materials in electrolytes by using electrochemical impedance spectroscopy (EIS). The measurement was carried out after the open circuit voltage was stabilized. Finally, Additives in ionic liquid based electrolytes are optimized for the best performance of DSC.

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발표종류: 포스터, 발표일시: 금 15:00~17:00

## **Enlargement of DSC sub-module and development of fabrication process by reducing efficiency loss for high-performed DSCs**

이현정, 이경주

현대하이스코 환경에너지연구팀

Dye-sensitized solar cells (DSCs) based on titanium oxide ( $\text{TiO}_2$ ) have been widely investigated as a new type of solar cell because of low production cost, simple structure, and competitive efficiencies. But although efficiency of test cell has been achieved up to 12%, when it turns to module, efficiency decreases dramatically. To overcome these problems, enlargement of sub-module and development of fabrication process for reducing efficiency loss have studied. In this study, we fabricated DSC sub-modules by screen printing method. The silver grid has applied to reduce sheet resistance of conducting glass. The sheet resistance measurement carried out by 4-point probe machine depending on grid structures of conduction glass. Energy conversion efficiency were measured by solar simulator under AM 1.5 condition.



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발표종류: 포스터, 발표일시: 금 15:00~17:00

## Thickness Effect of in-situ Prepared PbS/Polymer Composite Films for Hybrid Solar Cells

곽은주, \*우성호, 김화정, 김영규

경북대 화학공학과 \*대구경북과학기술연구원 나노바이오연구부

Among various energy conversion sources, solar cells are understood as one of the most viable and clean conversion media when it comes to their feature of direct conversion of photons (solar light) into electricity without generating high temperature steams. Although inorganic solar cells take initiatives in solar energy markets, most of their applications are limited to electrical power plants fixed on lands and/or buildings. In terms of organic solar cells, though their efficiency is still inferior to the inorganic solar cells, their applications are expected to be extended toward mobile and indoor applications. However, the stability of organic solar cells is still in doubt so that advanced approaches should be followed for the commercialization of organic solar cells. In our laboratory, we have concentrated on the development of hybrid solar cells because they could take advantages from both components (organic materials could provide low-temperature processes and flexibility/light-weight, while inorganic materials could secure the reliability of devices). Hence, we employed a lead sulfide (PbS) nanoparticle as the inorganic component. In particular, we synthesized the PbS nanoparticles in-situ in the presence of semiconducting polymers. In this presentation, we report the thickness effect of the PbS/polymer composite films on the performance of hybrid solar cells.

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발표분야: 환경에너지

발표종류: 포스터, 발표일시: 금 15:00~17:00

## Effect of Nitrogen-containing Carbon Spheres on Carbon Dioxide Adsorption

장동일, 박수진

인하대 화학과

In this study, we prepared the nitrogen-containing carbon spheres with mesopore processed by a facile polymerization-induced colloid aggregation method including carbonization in order to investigate the characterization and the effect on their carbon dioxide adsorption behaviors. The nitrogen contents of the mesoporous carbon sphere were characterized using XPS. The textural properties of the prepared mesoporous carbon sphere were investigated by  $N_2/77\text{ K}$  adsorption isotherms by Brunauer-Emmett-Teller (BET) equation. The carbon dioxide adsorption capacities of the prepared mesoporous carbon sphere were investigated by the amounts of carbon dioxide adsorptions at 298 K and 1.0 atm. Our results showed that the prepared mesoporous carbons have a high specific surface area, resulting from their uniform large meopores. The prepared mesopore carbons were highly effective for the capture of carbon dioxide adsorption capacities due to the increasing the affinity of the basic funtionalties of adsorbent surface to acidic carbon dioxide. Consequently, texture and surface chemistry of the carbon materials influenced the carbon dioxide adsorption performance of the adsorbents.

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발표종류: 포스터, 발표일시: 금 15:00~17:00

## Indirect Contact Bio-transformation of Lepidocrocite and the Role of Electron Transfer Mediator

정준영, 배성준, 이우진

KAIST 건설및환경공학과

Iron reducing bacteria shewanella putrefaciens CN 32 has been known to bio-transform Fe (III) bearing soil minerals into Fe (II) bearing soil minerals in direct and indirect manners. As a direct method, enzymes located interior of a cell or inside a membrane and a nano-wire involve in bio-transformation process. On the other hand, Chelator and electron transfer mediator can indirectly incorporate biotransformation as well. We have examined the effects of indirect reducing agent, ETM, on biotransformation. As the ETM, Anthraquinone 2 carboxyl acid was used in the biotransformation of lepidocrocite. The setup of a membrane filter enabled a reactor to prevent bio-transformation process via enzyme and nano wire, and let only ETM move through the membrane filter. In this system, the sole effect of ETM could be studied on bio-transformation of lepidocrocite. Without direct contact between lepidocrocite and shewanella, concentration of Fe (2) increased, and a gradual change in color of the soil mineral appeared. X-Ray Diffraction graphs were analyzed to identify the bio-transformed soil mineral, and transmission electron microscope image was obtained to observe the change in crystallization of bio-transformed soil mineral.

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발표분야: 환경에너지

발표종류: 포스터, 발표일시: 금 15:00~17:00

## **The effect of electron transfer mediator on the transformation of biogenic soil minerals**

배성준, 정준영, 이우진

KAIST 건설 및 환경공학과

Recently, the transformation of biogenic Fe<sup>2+</sup> soil minerals from amorphous Fe<sup>3+</sup> and/or Fe<sup>3+</sup> bearing soil minerals by iron reducing bacteria (e.g., *Geobacter*, *Shewanella*.) has been extensively studied in manner of bio-abiotic interaction. It has been known that type of electron transfer mediators (ETMs) significantly affect to biotransformation of soil minerals as a side of reduction kinetic and formation of biogenic particle. The effect of synthesized ETMs and biogenic ETMs on the formation of biogenic soil minerals has been examined to identify the formation mechanism. *Shewanella putrefaciens* CN32 and lepidocrocite ( $\gamma$ -FeOOH) were used as a representative of iron reducing bacteria and Fe<sup>3+</sup> contained soil mineral, respectively. Basically, the 0.5 M HCl extractable Fe was significantly increased when sodium lactate and PIPES were used as an electron donor and buffer system which showed that the formation of new biogenic soil minerals. The sample used synthesized ETMs (9,10-anthraquinone-2-carboxylic acid (AQC) and 9,10-anthraquinone-2-sulfonate (AQS)) showed the formation of green rust in the presence of PIPES, lactate and phosphate while the formation of vivianite was detected in the sample used biogenic ETMs (riboflavin, flavin adenine dinucleotide (FAD) Flavin mononucleotide (FMN)) in the same condition. In addition, new type of biogenic soil minerals were formed in the sample condition used biogenic ETMs in the absence of phosphate.

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발표분야: 환경에너지

발표종류: 포스터, 발표일시: 금 15:00~17:00

## Analysis of Produced Semiconductor By-Product by Waste Gas Treatment

김동호, 김태호, 권수한

충북대 화학과

반도체 공정에서의 폐가스 처리는 대기 환경의 측면에서 매우 중요한 문제이다. 대기 오염 물질 저감을 위해 사용되는 장비와 방법에 대한 효율성을 파악하는 것은 문제 해소를 위한 일부 접근 방법이다. 따라서 대상 오염원 포획 및 제거의 효율성을 확인하기 위하여 폐가스 처리에 따라 생성된 부산물의 분석이 반드시 이루어져야 한다. 본 연구에서는 실제 공정에서 발생한 부산물을 수집하여 분석이 이루어졌으며, 공정에 사용된 가스는  $\text{SiH}_4$ ,  $\text{NH}_3$ ,  $\text{NF}_3$  이다. 또한 가스는 가열-습식 복합 방식, 플라즈마-습식 복합 방식을 통해 처리되었으며, 분석 결과  $\text{CaSiF}_6$ ,  $(\text{NH}_4)_2\text{SiF}_6$ ,  $\text{CaCO}_3$ ,  $\text{SiO}_2$  가 검출되었다. 이를 바탕으로 각 성분의 포집 효율 향상을 위한 최적화 연구가 진행되어야 하겠다. 본 연구는 (주)뉴프로테크, Adixen (알카텔진공코리아)의 지원으로 이루어졌다.

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## The Influence of Water for the Product in Waste Gas Treatment Equipment

김동호, 권수한

충북대 화학과

반도체 공정에서의 폐가스 처리 후 부산물 생성은 필연적인 결과이다. 처리 공정에서 장비에 유입되는 수질에 의해 생성되는 부산물의 성분은 변할 수가 있으며, 실제로 분석 결과에서 공정 가스와 관계없는 성분이 검출되기도 하였다. 본 연구는 실제 반도체 업체를 대상으로 진행되었으며, 수질개선을 통한 폐가스 처리 장치의 성능 유지와 그에 따른 대기 오염 방지를 목적으로 하였다. 수질 개선을 위해 활성기, 이온교환 방식을 적용하였으며, ICP-OES, IC, FT-IR 을 사용하여 수질 분석되었다. 그 결과, 연수기 적용 후 장비에 영향을 주는 Ca 의 농도가 약 99.5 % 감소한 것을 확인하였다. 본 연구는 (주)뉴프로텍, Adixen (알카텔진공코리아)의 지원으로 이루어졌다.

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## Reductive capacity of soil minerals for Uranium(VI)

신영호, 이우진

KAIST 건설 및 환경공학과

우라늄은 원자력 발전소 및 군사시설을 비롯한 다양한 산업분야에서 원료물질로서 널리 사용되고 있으나, 우라늄의 radiotoxicity는 체내 유입 시 백혈병, 암 및 유전변이를 비롯한 치명적인 질병을 야기하므로 이와 같은 악티늄족 방사성 원소의 사용, 정제 및 폐기, 관리에는 극심한 주의가 요구된다. 특히, 방사성 폐기물 저장소 및 발전소 인근 지역에서는 사용자 부주의 및 시설 노후화로 인한 우라늄 누출 국내/외 사고 사례가 보고되고 있으며, 이로부터 방사성 물질로 오염된 토양 및 지하수 복원을 위해서는 이동성이 높은 6가 우라늄(U(VI))을 4가 우라늄(U(IV))으로 환원시켜 안정화 및 고정화를 통한 오염확산 방지가 요구된다. 본 연구에서는 U(VI) 환원제로써 경제성을 갖춘 철 함유 토양광물들을 이용하여, 각 토양 광물들의 우라늄 환원능을 측정하고 상호 비교를 하였다. 철 함유 토양광물으로써 magnetite( $\text{Fe}_3\text{O}_4$ ), nZVI( $\text{Fe}(0)$ ), mackinawite( $\text{FeS}$ ), pyrite( $\text{FeS}_2$ )를 사용하여  $\text{Fe}(0)$ 과  $\text{Fe}^{2+}$ 가 U(VI)환원에 미치는 영향을 파악하고자 하였으며, uranyl nitrate hexahydrate( $\text{UO}_2(\text{NO}_3)_2 \cdot 6\text{H}_2\text{O}$ )을 U(VI) standard solution으로 사용하였다. 반응시간에 따른 aqueous phase 내 U(VI) 총 농도 변화는 ICP-AES (Inductively Coupled Plasma Atomic Emission Spectroscopy)를 이용하여 측정(예, magnetite를 이용한 경우 8시간 내로 대략 90%의 U(VI)가 제거됨)하였다. 광물표면에 형성된 화합물을 XPS(X-ray Photoelectron Spectroscopy) 및 XRD(X-ray Diffraction)로 분석하여 U(VI) 환원여부를 규명하였으며, SEM(Scanning Electron Microscope)분석을 통해 U(IV) 입자의 크기 및 morphology를 확인하였다. 더불어 U(VI) 및 토양광물간의 redox 반응 메커니즘을 추적하고자 geo-chemical modeling program인 PHREEQC을 이용하여 시뮬레이션을 실시하였다. 본 실험 결과는 우라늄에 의해 오염된 토양 및 지하수환경 복원기술 개발에 관한 기초정보를 제공할 것이며, 더불어 방사성폐기물 관리기술 분야로 적용 가능할 것으로 기대된다.

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## lective removal of Halogenated organic contaminants including DBPs using ZVI and catalysts

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영가금속 및 영가이중금속을 이용하여, 정수장에서 염소소독시 발생하는 소독부산물의 환원분해연구를 하였다. 각 소독 부산물의 구조 및 화학적 특성에 따른 반응성을 조사하여 그 경향성을 연구 하였다. 환원분해 대상 모델 소독부산물로는 클로로아세트니트릴을 선정하였다. 이 부산물은 수돗물 염소소독이나 음용수 소독과정에서 유기 전구체로부터 생성되는 것으로 알려져 있으며 생물 독성이 높다. 연구결과 각 영가금속은 대상물질인 소독부산물에 대하여 성공적인 환원분해능을 보였으며, 염소화정도 및 촉매사용에 따른 반응성차이를 확인하였다. 기존 연구결과와 유사하게 영가금속은 단계적 탈염소경향을 보이는 반면 촉매를 사용한 경우 탈염소환원반응이 단축되는 것으로 나타났다. 기존의 소독부산물생성저감을 위한 자연유기물제거 및 활성탄흡착을 이용한 유기물의 비선택적 전량제거와 달리 유독부산물을 선택적으로 제거하는 기술로 발전할 수 있을 것으로 판단된다.



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## Influence of Dissolved Organic Ligands on the Reactivity of Nano Zero Valent Iron(nZVI) for persistent explosive compounds degradation

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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 나노영가철(nZVI)의 반응성 및 반응정도에 유기리간드가 미치는 영향에 대해 조사하였다. 유기리간드를 나노영가철 수용액에 첨가하였을 경우 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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## Complexation of Cobalamin (II) with Nucleophile Enhanced Reductive Dechlorination of Tetrachloroethene by Mackinawite

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Batch experiments were performed to verify the significant interaction between cobalamin (III) and mackinawite (FeS) on the reductive dechlorination of tetrachloroethene (PCE). Cobalamin (III) can be produced by sulfate-reducing bacteria, methanogenic and acetogenic bacteria at anaerobic condition. Interaction between cobalamin (III) with FeS significantly enhanced reductive transformation of PCE. Approximately 80% of PCE was degraded by FeS-cobalamin(III) suspension, while only 10% of PCE was degraded by FeS and Fe(II)-treated FeS suspension in 12 hrs at pH 8.3. Formation of cobalamin(II)-sulfide (CoS) and hydroxocobalamin(II) (Co(OH)<sub>2</sub>) were detected at 784 eV and 431 eV on FeS surface by X-ray photoelectron spectroscopy analysis in FeS-Cobalamin(III) sample. This finding suggests that the reduction of cobalamin (III) to cobalamin (II) and complexation of cobalamin (II) with sulfide (S<sup>2-</sup>) and hydroxyl (OH<sup>-</sup>) ions are the main important reaction mechanisms for acceleration of reductive dechlorination rate of PCE in FeS-cobalamin(III) system. This study revealed that the formation of CoS and Co(OH)<sub>2</sub> as potential catalysts in enhancement of reductive dechlorination of PCE by FeS in reducing environments. This study provides significant findings on the reactivity of complexation of reduced cobalamin species with nucleophiles as a significant catalyst to enhance reductive dechlorination of chlorinated organic compounds in reducing environment.

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## Investigation on enhanced oxidative degradation of trichloroethylene by nano and microscale zerovalent iron in the presence of copper

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KAIST 건설 및 환경공학과

Characterization on the enhanced reactivity of zerovalent iron (ZVI) in the presence of copper was studied. Surface on ZVI was hydrated by pH 3 deaerated deionized water (DDIW) and copper(II) spiked after hydration was bound to ZVI surface, resulting in oxidative dissolution and release of considerable amounts of ferrous in case of both nano and microscale ZVI (nZVI and mZVI). Interestingly, the amounts of ferrous ion (1, 10, 20 mM) produced by copper binding were directly proportional to the amounts of copper(II) ion (1, 10, 20 mM) introduced into the reaction system at initial pH 3 which was adjusted by 3 M H<sub>2</sub>SO<sub>4</sub>. However, ZVI suspension without copper just produced a range of ferrous concentration (0.35 ~ 0.4 mM). Relatively large amounts of ferrous ion in ZVI suspension with Cu compared to that in sole ZVI suspension might be the reason why the Fenton reaction by bimetallic system showed better degradation patterns (Cu/nZVI Fenton, 95%; Cu/mZVI Fenton, 99%) than that by sole ZVI system (nZVI Fenton, 25%; mZVI Fenton, 10%) within 10 min. Differences in reactivity and reaction continuity for each size of ZVI with copper could be explained by surface analysis (SEM/EDS).

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## Development of Lipase Immobilized Polymer-Support Catalyst for Bio-Diesel Application

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서울대 화학생명공학부

Bio-diesel, derived from triglycerides including vegetable oils, animal fats, has drawn much attention as an alternative fuel to replace petroleum based diesel. For the industrial bio-diesel production, homogeneous acid or base catalysts have been generally used. But this process requires additional separation steps to remove the catalysts and additional distillation process and has lots of other disadvantages, not to mention about the side reactions. In this sense, enzyme catalyzed trans-esterification process is very attractive for the bio-diesel production. In this work, we prepared ionic liquid immobilized polystyrene bead as a solid-support for the immobilization of lipase. We will report on the hydrophobic effect of anions of the immobilized ionic liquid for the enzymatic trans-esterification of fatty acid for bio-diesel production.

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## Characterization of extractable organic matter as potential hydrate nucleator

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KAIST 건설 및 환경공학과 \*KAIST 건설및환경공학

Marine sediment core samples collected from a gas hydrate deposit site (Ulleung Basin (UB), East Sea, South Korea) were analyzed for sedimentary organic component to identify the role of SOMs (sediment organic matter) on the formation of CO<sub>2</sub> hydrate. Three fractions of sediment organic matter were obtained from different extraction procedures. Both nonhumic and humic substances were assumed to be found in the samples. Dichloromethane: methanol (1:1) was used to extract the polar component and dichloromethane-only was used to extract the non-polar component. An alkaline (using NaOH) extraction was used to extract the humic fraction. Chemical characterization with CHNS analyzer, proton nuclear magnetic resonance (<sup>1</sup>H NMR), Fourier transform infrared spectroscopy (FTIR), and ultra performance liquid chromatography-electrospray ionization-mass spectrometry (UPLC-ESI-MS) confirmed the existence of significant amount (3.4% organic carbon) of different SOMs in UB sediment samples. We detected SOMs with aliphatic and aromatic ring structures in all sediment extracts but SOMs with amide structures are only found in sediment extracts by alkaline solution. SOMs with oxygen-containing compounds were detected in the polar extracts. UPLC-ESI-MS analysis proposes several molecular formulas with relatively high molecular weights. These chemical fragments may have reoriented with water molecules forming an ideal hydrogen bonding network in a hydrate-like domain (e.g., hexagonal-like or polymeric structures) large enough to be potential sites for nucleation.

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## Synthesis of ethyl lactate from ammonium lactate solution by coupling solvent extraction with esterification

palraj kasinathan, 곽효진, \*황영규, \*\*장종산

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Ethyl lactate was synthesized selectively from aqueous ammonium lactate by coupling solvent extraction with esterification with ethanol. When ammonium lactate reacted directly with ethanol without solvent, the ethyl lactate yield was very low due to significant formation of byproducts such as oligomer and lactamide (Conv. 70%, Sel. 10% at 10 h). The significant improvement in ethyl lactate yield was obtained when lactic acid was extracted from ammonium lactate in tributyl phosphate and then it reacted with ethanol, where oligomer formation was decreased greatly (Conv. 78%, Sel. 95% at 10 h). Compared with the traditional method including acidulation of calcium lactate, extraction, and esterification, the present technique is potentially more economical since it enhances not only the productivity of lactic acid fermentation but also the efficiency of overall process from fermentation broth to ethyl lactate.

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## Photoelectrochemical Study on Hematite/TiO<sub>2</sub> Nanotubes

전태화, \*박현웅

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Nanocrystalline hematite particles ( $\alpha$ -Fe<sub>2</sub>O<sub>3</sub>) were electrodeposited on the TiO<sub>2</sub> nanotube (TiNT) arrays that were fabricated via anodization of Ti foils. The short pre-contact time (1 h) of aqueous ferric ions (Fe<sup>3+</sup>) on TiNT resulted in formation of hematite particles selectively on the mouth surface of TiNT (hematite@1h/TiNT) while the long pre-contact time (24 h) resulted in complete filling of the TiNT inside and an even full-covering of the TiNT top surface with the hematite particles (hematite@24h/TiNT). For comparison, hematite particles were also electrodeposited on TiO<sub>2</sub>-nanoparticulate films obtained via oxidative annealing of Ti foil resulting in hematite-fully covered TiO<sub>2</sub> nanoparticles (hematite/TiNP). Photoelectrochemical (PEC) study with AM 1.5 light (UV + Vis) indicated that the PEC activity of TiNT decreased by ca. 40% and almost completely vanished when hematite covered the full surface of TiNT (hematite@24h/TiNT) and loaded on the mouth surface of TiNT (hematite@1h/TiNT), respectively. The relatively higher PEC activity of hematite@24h/TiNT was further observed under varying visible light conditions (400 nm <  $\lambda$  < 500 nm). Hematite/TiNP also has ca. 40%-reduced PEC activity as compared to TiNP under AM 1.5 light, the tendency of which is similar to hematite@24h/TiNT. Photocatalytic (PC) activities of TiNT and hematite/TiNT for degradation of aqueous phenol under AM 1.5-light were also compared, which indicates that the PC activity of TiNT vanishes almost completely with hematite@1h/TiNT while it is recovered at a moderate level with hematite@24h/TiNT. All these PEC and PC behaviors of TiNT and hematite/TiNT were discussed in terms of hematite-induced charge recombination due to an energy level mismatch between TiO<sub>2</sub> and hematite, as well as surface-specific photo-activity of TiNT (i.e., mouth surface vs. inter-wall and/or underlying base layer). Various surface analysis techniques (XRD, XPS, TEM, UV-vis diffuse reflectance) were employed to understand the surface states of TiNT and hematite/TiNT. Finally, more detailed charge transfer mechanism was proposed.

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## Synthesis of CuInS<sub>2</sub> nanocrystal inks for low-cost thin film solar cells

조진우, \*김웅, \*\*민병권

고려대 신소재공학과 \*고려대 신소재공학부 \*\*KIST 청정에너지연구센터

Recent advances in colloidal science are having a dramatic impact on the development of next generation low-cost and high-efficiency solar cells. Simple and safe solution phase synthesis that yields monodisperse, passivated, non-aggregated semiconductor nanocrystals of high optoelectronic quality have opened the door to several routes to new photovoltaic devices which are currently being explored. In one route, colloidal semiconductor nanocrystal “inks” are used primarily to lower the fabrication cost of the photoabsorbing layer of the solar cell. In this study, we present a facile solution synthesis of chalcopyrite CuInS<sub>2</sub> nanocrystals and demonstrate that inks based on. These nanocrystals were redispersed in organic solvent with a suitable viscosity to use as an ink. After spraying and annealing the film was selenized in Se/Ar vapor environment to make highly crystalline film. The structural and optical properties of the chalcopyrite nanocrystals and films will be discussed in the presentation.



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## Plasmonic dye-sensitized solar cell fabricated by a Au-TiO<sub>2</sub> powder

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One of the promising applications of TiO<sub>2</sub> incorporated with gold nanoparticles would be a dye sensitized solar cells (DSSC) where mesoporous TiO<sub>2</sub> films were generally used for adsorbing the dye molecules and transporting photogenerated electrons. TiO<sub>2</sub> incorporated with gold nanoparticles has been attracted due to the typical optical properties of gold nanoparticles known as a localized surface plasmon resonance. In this study, We synthesized gold catalysts supported on TiO<sub>2</sub> that were prepared by a deposition-precipitation (DP) method. And then, Au-TiO<sub>2</sub> catalysts are applied for Dye-sensitized solar cell. Especially, in order to investigate the effect of gold nanoparticles on DSSC various Au-TiO<sub>2</sub> films were applied instead of TiO<sub>2</sub>, and those optical properties and solar cell performances were compared. The details will be discussed in the presentation.

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## Printable CIGS thin films for solar cell applications

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$\text{CuIn}_x\text{Ga}_{1-x}(\text{Se}_y\text{S}_{1-y})_2$  (CIGS) has been considered to one of the most promising materials for solar cell applications due to its high absorption coefficient, appropriate band-gap, and long-term stability. The obstacles of the current CIGS thin film solar cells for commercial applications may be relatively difficult fabrication procedure and high processing costs related with vacuum based techniques. Herein, we suggest a simpler and lower cost synthetic method of CIGS thin film by applying a paste coating methode. In this method the paste containing Cu, In, Ga precursor mixtures was firstly prepared followed by being printed on conducting glass substrates and then annealing in  $\text{H}_2\text{S}/\text{Ar}$  and/or Se vapor environment. With this method we applied CIGS thin films to both substrate and superstrate type solar cell architectures using Mo coated soda-lime glasses and  $\text{TiO}_2$  coated FTO glasses, respectively. The compositional and structural characteristics of the films were investigated by various analysis techniques including XRD, SEM and EPMA. The details will be discussed in the presentation.

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## Electrocatalytic Remediation of Aqueous Phenol Using Multi-Layered BiOx-TiO<sub>2</sub> Anodes

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Multi-layered BiOx-TiO<sub>2</sub> anodes (5 kinds) were studied on their electrocatalytic activities for degradation of aqueous phenol and their activities were compared with those of Ta-IrO<sub>2</sub> and Sb-SnO<sub>2</sub> anodes. Each anode has been fabricated via layer-by-layer coats on Ti foil with different element compositions (Ir, Ta, Sb, Sn, Bi, and Ti) and tested in three different supporting electrolytes (Na<sub>2</sub>SO<sub>4</sub>, NaClO<sub>4</sub>, and NaCl). As compared to Sb-SnO<sub>2</sub> anode, BiOx-TiO<sub>2</sub> anodes were found to be less effective in degradation of phenol in Na<sub>2</sub>SO<sub>4</sub> and NaClO<sub>4</sub> electrolytes; yet in NaCl their electrocatalytic activities become similar with or greater than that of Sb-SnO<sub>2</sub> anode. Also, irrespective of anodes, the degradation of phenol was highly accelerated in NaCl along with generation of various chlorinated phenols. More detailed kinetic comparison and mechanistic interpretation depending on anodes and electrolytes will be presented.

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## **Solar Hydrogen Production in Water Using Dye-Sensitized Carbon Allotropes**

정혜원, 박현웅

경북대 물리 및 에너지학부

This study demonstrates that dye-sensitized carbon allotropes can be used as a photocatalyst for hydrogen production from water. In order to compare 5 kinds of carbon allotrope for their dye-sensitization effects, we have employed powder samples of activated carbon (AC), carbon nanofibers (CNF), multi-walled carbon nanotubes (MWNT), single-walled carbon nanotubes (SWNT), and graphite (GP). For simplicity in comparative experiments, a well-known organic dye, Eosin Y (EY) was adsorbed to the carbon allotropes and AM 1.5-light was irradiated to the aqueous suspensions of EY-sensitized carbon allotropes in the presence of an electron-donating triethanolamine (TEOA). It has been found that MWNT is the best materials among the five carbon allotropes primarily due to the highest conductivity and the largest amount of EY adsorbed. Various experiments were conducted including optimization of the sensitized system for hydrogen production, EY adsorption/desorption, stability of EY, and comparison of carbon allotropes for their conductivities and surface areas, and will be presented.

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## **Rice straw biomass-fueled air-cathode single chamber microbial fuel cell for power generation**

최찬수

대전대 응용화학과

A single chamber MFC equipped with Nafion® ionomer covered air-cathode was adapted to evaluate the flexibility of using rice straw biomass as a fuel for power generation at first time. As one kind of the most abundant biomasses on earth, rice straw was usually pretreated to be used to generate ethanol. Organic matters in rice straw hydrolysate could be an alternative fuel for microbial fuel cells. However, no such research has been reported. In this study, a maximum power density of  $137.6 \pm 15.5$  mW/m<sup>2</sup> cathode was generated in an air-cathode microbial fuel cell, and increased to  $292.3 \pm 7.9$  mW/m<sup>2</sup> after the solution conductivity was adjusted from 5.6 mS/cm to 17 mS/cm. Coulombic efficiency of the rice straw hydrolysate fueled microbial fuel cell was in the range of  $8.54 \pm 2.06$  % to  $17.89 \pm 0.91$  %. This study may reveal a new energy resource utilizing rice straw biomass.

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## Synthesis of Cadmium-Incorporated Iron Oxide Films and Their Photoelectrochemical Performances for Water Oxidation

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*School of Energy Engineering*

Cd-incorporated nanocrystalline hematite films ( $\text{Cd-Fe}_2\text{O}_3$ ) supported on conducting glass have been prepared via co-electrodeposition of aqueous Fe(III) and Cd(II) with varying Cd:Fe atomic ratios (0 ~ 0.15) and optimized for their photoelectrochemical (PEC) performances under AM 1.5-light. Surface analysis indicates that the Cd co-deposition increases the hematite ( $\alpha\text{-Fe}_2\text{O}_3$ ) particle size from ca. 50 nm to 70 ~ 100 nm due to interparticle agglomeration despite the similar film thickness of ca. 1.7  $\mu\text{m}$  with high porosity whereas it decreases the overall UV-Vis absorbance of hematite with increasing Cd atomic content. X-ray photoelectron spectroscopic study suggests that Cd incorporation shifts the binding energy of oxygen atoms to lower energy direction whereas it did not affect the binding energy of Fe 3d, implying that Cd exists mainly as CdO and/or  $\text{Cd(OH)}_2$  on the hematite surface. When Cd of 5 ~ 8 atomic % was co-electrodeposited, the photocurrent of hematite film was significantly enhanced by a factor of ca. four at  $E = 1.23 \text{ V}_{\text{RHE}}$  under AM 1.5-light and such enhancement was maintained even under the irradiation condition of  $\lambda \sim 665 \text{ nm}$ . Electrochemical impedance spectroscopic analysis further revealed that the flat band potential of hematite was shifted by ca. -30 mV to negative potential direction and the charge transfer resistance ( $R_{\text{ct}}$ ) was significantly reduced by Cd incorporation. On the basis of through surface and photoelectrochemical study, electrodeposited Cd was speculated to be mostly present on the hematite surface as forms CdO and  $\text{Cd(OH)}_2$ , which play multiple roles in generating the Cd-induced effects. Detailed surface analyses, optimization for preparation condition of hematite films, and discussion for PEC behaviors were described