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장소: 송도컨벤시아

발표코드: **목1J1특별**

발표분야: 기조강연

발표종류: 특별강연, 발표일시: 목 11:00, 좌장: 도춘호

The Chemical Enterprise: Thinking and Acting Globally

Joseph S. Francisco

ACS President

We continue to see that accelerated technological, environmental, societal and financial drivers are pushing the chemical enterprise worldwide, and chemists working in it, to increasingly think and act globally. There are challenges and opportunities for our shared discipline and its enterprise. What are characteristics of a 'global-ready' chemistry practitioner? Do we have that new workforce of chemical scientists, engineers, and teachers capable of working with and across different cultures to tackle global societal challenges? What are the global knowledge and skill sets needed by universities, companies and research labs in our countries to be successful in a globally competitive research, development and innovation environment? For chemistry and the chemical enterprise to flourish, will it become normal for chemistry students, teachers, researchers and professionals to spend some part of the year in some one else's country? What is the role of the national chemical society to help enable this transnational mobility of chemists? Finally, how do we foster a greater public understanding and appreciation for the transformative power of chemistry? And to this end, how can we best leverage and extend the celebrations of the 2011 International Year of Chemistry?

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Searching for New Reactivity of Transition Metal Catalysts for the Efficient and Selective Organic Transformations

장석복

KAIST 화학과

It has been discovered that a highly efficient, mild, and practical multi-component reaction for the synthesis of amidines, amdies, and imidates, which are prominent structural motifs in numerous bio-active natural products, important pharmacophores, synthetic intermediates, and efficient coordinating ligands. The electron deficient character of the sulfonyl substituent induces that the triazolyl intermediate makes progress toward the ketenimine by electron rearrangement and releasing dinitrogen. A new strategy for the synthesis of condensed hetero- and carbocycles such as pyrroloindoles or fluorenes has been developed that involve Pd-catalyzed cyclization of readily available N-(2-halobenzyl)pyrroles and their phenyl derivatives. The reaction is proposed to proceed via successive oxidative addition of benzylic halides to Pd(0) followed by base-assisted aromatic C-H bond activation. Thus, a broad range of condensed cyclic products were obtained in good to excellent yields.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.References1) Park, E. J.; Kim, S. H.; Chang, S. J. Am. Chem. Soc. 2008, 130, 17268.2) Hwang, S. J.; Cho, S. H.; Chang, S. J. Am. Chem. Soc. 2008, 130, 16158.3) Cho, S. H.; Hwang, S. J.; Chang, S. J. Am. Chem. Soc. 2008, 130, 9254.4) Lee, J. M.; Park, E. J.; Cho, S. H.; Chang, S. J. Am. Chem. Soc. 2008, 130, 7824.5) Cho, S. H.; Chang, S. Angew. Chem., Int. Ed. 2008, 47, 2836.6) Cho, S. H.; Hwang, S. J.; Chang, S. Organic Syntheses 2008, 85, 131.6) Kim, M.; Kwak, J.; Chang, S. Angew. Chem. Int. Ed. 2009, 48, 8935.7) Cho, S. H.; Kim, J.; Lee, S. Y.; Chang, S. Angew. Chem. Int. Ed. 2009, 48, 9127.

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발표종류: 심포지엄, 발표일시: 금 14:00, 좌장: 장우동

Development of non-viral polymeric gene carriers

김원종

포항공과대 화학과

Gene therapy has been studied as an efficient tool for controlled regeneration or specific inhibition of tissue growth. In order to magnify the efficacy of gene therapy, development of powerful gene delivery carrier is essential issue as well as design of therapeutic gene. In this study, we developed various polymeric gene carriers for delivering therapeutic gene into specific cell or tissues. Physicochemical characterization of polymers was evaluated followed by gene transfection assay in vitro. In addition, we investigated the efficacy of gene carriers for delivering therapeutic gene in vivo.For development of target-specific gene carrier, dextran, a biodegradable natural polysaccharide, has been modified with cationic oligoamine, spermine. In addition, for achieving cell specific-targeting, galactosylated cucurbituril(galCB) was added to the cationic polysaccharides via host-guest interaction between spermine and galCB. For treatment of a vascular disease, hybrid polymer-superparamagnetic iron oxide nanoparticle was evaluated as efficient gene delivery vehicles in the presence of a magnetic field. In short incubation time, luciferase reporter proteins were effectively expressed by BPEI-SPION on tumor cells in the presence of magnetic field

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나노기술을 이용한 광역학 치료 기술 개발

나건

가톨릭대 생명공학과

서론 광감작제의 효과는 국부적으로 투여된 광감작제가 빛 자극을 받음으로 생기는 단분자 산소, 자유라디칼들 또는 과산화물질들과 같은 세포독성물질에 의해 생긴다. 이러한 광역학치료는 빛이 투과하지 못하는 크기가 큰 종양세포에는 적용이 어려우며 광감작제의 반감기때문에 시술 후 빛이 없는 환경에서 생활해야 하는 불편함이 있으며 종양으로의 축적이 어렵고 국부투여하지 않는이상 표적화 할수 없는 단점을 가지고 있다. 체내에 오랫동안 남아 부작용을 일으키며 시술시 효율이 떨어지는 문제를 극복하고자 암 세포로의 축적률과 표적률을 높이고 암세포 이외에서는 형광간섭으로 인한 광독성을 현저히 줄여주는 새로운 광역학치료 및 진단에 이용할 수 있는 나노 미립구를 개발하게 되었다. *재료 및 방법* 생체적합성 고분자에 암세포 표적화를 가지는 물질을 유기용매상에서 결합시킨 후 투석 및 동결건조를 통해 물질을 얻는다. 얻어진 물질에 광감작제를 여러가지 비율로 유기용매상에서 결합시킨 후 동결건조를 통해 물질을 얻는다. 그 후 ^{1}H-NMR 을 통해 암세포 표적화 물질의 합성비율과 광감작제의 합성비율을 분석한다. *결과 및 고찰* 전자 현미경을 통해 나노미립구의 모양도 확인하였고 크기는 대략 100~200nm 사이 였다. 광감작제의 자가형광을 띄는 성질을 이용하여 공초점현미경으로 시간에 따른 나노미립구의 세포내 위치를 확인하였으며 세포내에서 분해되는 현상과 대략적인 시간을 알 수 있었다. 감작제의 일항산소 생성능을 측정해본 결과에서는 화학적 개질을 하지 않은 광감작제와 화학적 개질을 시킨 광감작제의 일항산소 생성능에서는 큰 차이가 없기 때문에 나노미립구로 이용 시에도 치료적인 측면에는 큰문제가 없을것으로 예상했다. 실제 세포 독성실험결과 에서도 화학적 개질을 하지 않은 광감작제와 거의 동일한 치료효과를 가지는 것을 확인하였다.

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Preparation of nanoporous bioactive materials for bone tissue regeneration

윤희숙

한국기계연구원부설 재료연구소 엔지니어링세라믹연구그룹

Nanoporous bioactive ceramics with different nano-pore structures and compositions have been synthesized by a combination of supramolecular polymer templating and sol-gel processes. New synthetic techniques for fabricating hierarchically porous bioactive ceramics, containing nanopores, have been suggested, such as multi-polymer templating and a combination of polymer templating and rapid prototyping. The texture properties of hierarchically porous bioactive ceramics and their potential use in bone tissue regeneration have been characterized. The materials obtained contained 3 dimensionally well interconnected pore structures, ranging in size from nano to macro, with good bioactivity, and biocompatibility. We report our recent research results and demonstrate the potential applications of nanoporous bioactive ceramics in bone regeneration and other biomedical areas.

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Charge-conversional polyion complex for the efficient delivery of charged biomacromolecules into cytoplasm

이연, *Kazunori Kataoka

*서울대 화학부 *Department of Materials Engineering, the University of Tokyo*

For a highly efficient delivery method that offers serum stability and generality, we developed a polyion complex (PIC), which is based on a charge-conversional chemistry of citraconic acid amide and cis-aconitic acid amide. The citraconic acid amide and cis-aconitic acid amide have negative charges at normal physiological pH value of around 7, but they can be degraded rapidly to expose amines with positive charges at weakly acidic pH value of 5.5. Because the pH value in early endosome is around 5.5, the polymers with the citraconic acid amide and cis-aconitic acid amide moieties can show rapid charge-conversion responding to the early endosomal pH. By using the charge-conversional chemistry, we can prepare a charge-conversion polymer with endosome disruption activity, to transfect plasmid DNA on a hard-to-transfect primary cell line, HUVEC, with high efficiency and low toxicity. Moreover, membrane-impermeable proteins can be successfully delivered into live cytoplasm by a charge-conversional PIC micelle, which is composed of a charged block copolymer and temporarily charge-increased proteins. The charge-conversion chemistry provides a versatile method to change the charge density of biomacromolecules and reverse it to original one at endosomal pH.((References))1. Efficient delivery of bioactive antibodies into the cytoplasm of living cells by charge-conversional polyion complex micelles.(2010) Angew. Chem. Int. Ed. (accepted).2. Charge-conversional PIC micelles – an efficient protein delivery nanocarrier into cytoplasm. (2009) Angew. Chem. Int. Ed. 48: 5309-5312.3. Charge-conversional ternary polyplex with endosome disruption moiety: a technique for efficient and safe gene delivery. (2008) Angew. Chem. Int. Ed. 47: 5163-5166.

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Self-Assembled Hyaluronic Acid Nanoparticles for Cancer Imaging and Therapy

박재형

경희대 화학공학과

Hyaluronic acid (HA), a major component of extracellular matrix in our body, has been recieved attention because of its biocompatiblilty and uinque biological characteristics. In particular, many researches have demontrated the potential of HA as the targeting moiety for drug delivery in cancer therapy because cancer cells often overexpress the HA receptor, CD44, on their surfaces. Recently, several HA-drug conjugates have been developed as macromolecular prodrugs, in which the drug conjugates become active upon release from the backbone of HA. Also, HA has been chemically or physically anchored onto various nanoparticles imbibing drugs. In this study, we aimed to develop amphiphilic HA conjugates by chemical conjugation of hydrophobic bile acid to hydrophilic HA. This amphiphilic HA conjugates could be capable of being self-assembled to form a stable nanoparticle strcutre in an aqueous environment. The chemical structure, particle size, surface charge, morphology of HA-NPs were studided. Also, the cellular uptake profile of HA-NPs were evalulated in vitro cell culture system. Thereafter, in vivo characteristics, such as time-dependant biodistribution and tumor targeting ability were evalulated in tumor-bearing mice by using non-invasive and live imaging system.

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Multivalent Signaling across G Protein-Coupled Receptors from Poly(amidoamine) Dendrimer Conjugates

김윤경, *Béatrice Hechler, **Zhan-Guo Gao, **Athena M. Klutz, *Christian Gachet, **Kenneth A. Jacobson

*한국생명공학연구원 바이오나노연구센터 *INSERM U.311, EFS-Alsace and Université Louis Pasteur, Strasbourg, France **Molecular Recognition Section, Laboratory of Bioorganic Chemistry, National Institute of Diabetes and Digestive and Kidney Diseases, National Institutes of Health, Bethesda, Maryland 20892, U.S.A.*

Small molecule ligands of G protein-coupled receptors (GPCRs) bind primarily at their heptahelical transmembrane domain to induce various intracellular signaling pathways. Diseases relevant to the adenosine receptor (AR), a GPCR, include cancer, arthritis, thrombosis, ischemia, and sleep disorders. In an effort to enhance the therapeutic potential of GPCR ligands through the multivalent effect, multiple copies of CGS21680–a nucleoside-based agonist of A_{2A} AR–were covalently attached to the surface of fluorescently labeled poly(amidoamine) (PAMAM) dendrimers. These dendrimer conjugates were further derivatized with varying numbers of PEG550/PEG750/PEG2000, in order to improve water-solubility and biocompatibility and to systematically investigate the influence of PEG chains on the biological activities of the surface-bound ligands on a common macromolecular carrier. All dendrimer conjugates were purified by size exclusion chromatography and characterized by ^{1}H NMR and MALDI MS. In radioligand binding assays, some PAMAM-PEG-CGS21680 conjugates showed enhanced subtype-selectivity at the human A_{2A} AR compared to the monomeric ligands of comparable affinity. The functional potency was measured in the A_{2A} AR-mediated activation of adenylate cyclase and inhibition of ADP-induced platelet aggregation. Interestingly, the dendrimer conjugate bearing 11 PEG750 chains (out of theo. 32 amino end groups) and 14 nucleoside moieties was 5-fold more potent than that with 4 PEG2000 chains and 21 nucleosides, although the binding affinities of these two compounds were similar. We envision that the high potency value shown by a relatively small ($\leq$10 nm) multivalent ligand might have further benefited from receptor clustering and oligomerization upon binding. This study

demonstrates i) the improvement of overall pharmacological profiles by using multivalent dendrimer conjugates, and ii) the possible use of short PEG chains to design carriers that involve ligand-receptor interactions.

대 한 화 학 회
THE KOREAN CHEMICAL SOCIETY

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Organic Syntheses and Properties of Stabilized Conjugated Polymers for AMOLEDs

서홍석

부산대 화학과

Conjugated polymers with a stabilized blue emission are of importance for the realization of full-color displays using polymer light-emitting diodes. Several types of novel conjugated polymers with stabilized electroluminescence (EL) emission are reported. Poly(2,6-(4,4-bis(2-ethylhexyl)-4*H*-cyclopenta[*def*]phenanthrene)) (PCPP) is a new class of blue-emitting polymers utilizing a new back-bone. This material emits a stabilized, efficient blue EL without exhibiting any peak in the long wavelength region (green region) even after prolonged annealing for 18 hours at an elevated temperature of 150°C in air. In PININE, the vinylene group was cyclized using two 5-membered rings to prevent the oxidation of the vinylene group. While poly(*p*-phenylenevinylene) derivatives show significantly blue-shifted and decreased peaks of UV-vis, blue-shifted maximum peaks of photoluminescence (PL) after irradiation with white light in air, and blue-shifted maximum peaks of EL after operation of the device, PININE shows stable spectra of UV-vis, and PL, and EL under the same conditions.

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Terminally-crosslinked sulfonated poly(ether sulfone)s as novel polymer electrolyte membranes for both high temperature PEMFC and DMFC applications

김태현, roshni

인천대 화학과

Sulfonated aromatic polymers have been widely studied as one of the alternatives to Nafion for PEMFC and DMFC applications. However, a high degree of sulfonation degrades the physical properties of the humidified polymers. Crosslinking has often been used as an efficient means to enhance physical and mechanical properties of the highly sulfonated membranes, but a reduced proton conductivity was inevitably accompanied for most cases of the crosslinked membranes. In a fusion of the benefits of both sulfonated aromatic polymers and crosslinking, we have recently introduced an azide-assisted thermally crosslinked polymer system where the terminal crosslinking has brought a balanced hydrophobic nature for the highly conductive polymer network. Unlike other thermally-crosslinked membranes, our crosslinked sulfonated poly(ether sulfone)s (PESs) displayed an exceptionally high proton conductivity especially at elevated and hydrated conditions, and yet maintained most of their structural integrity. Synthesis and properties of the terminally-crosslinked PESs will be detailed, and a dramatic conductivity enhancement of our crosslinked membranes under hydrothermal conditions will also be described.

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Self-organized polymeric anode with tunable work function for flexible organic device applications

이태우

포항공과대 신소재공학과

Since ultra-thin and flexible electronic devices are one important form of future electronic devices, stable flexible anodes in organic devices such as organic light emitting diodes (OLEDs) and organic photovoltaic (OPVs) should replace the brittle and expensive indium-tin oxide (ITO) anode on polymeric substrates. Although many approaches have been reported so far, the work functions of the anodes were still low and thus hole injection or extraction in OLED and OPVs becomes still problematic. Therefore, work-function-tunable flexible anode should be developed for flexible devices. We tuned the work function of the polymeric anode of poly(4-styrenesulfonate) doped poly(3,4-ethylenedioxythiophene) (PEDOT/PSS) by using a perfluorinated ionomer (PFI) with which an additional hole injection or extraction layer in OLED and OPVs is not necessary. The green emitting small molecule OLEDs based on our polymer anode showed a very high luminous efficiency of ca 18 cd/A. We will show a successful replacement of the ITO with our polymeric anode in OPVs. Our polymeric anode is very useful in various organic devices due to its flexibility and work-function tunability.

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A Novel Ceramic Coated Separator for Enhanced Safety of Li-Ion Battery

김종훈

(주)LG화학기술연구원 Battery 연구소

The lithium-ion battery separator is a micro-porous membrane placed between a cathode and a anode, and its main functions are to physically isolate two electrodes and so that no electrons can flow in between in a point view of the safety of the battery. Specially, the internal short-circuits caused by protrusions on the electrode surface either by unavoidable metallic impurities or by the growth of lithium dendrites during battery operation has been the most fatal to battery safety. Furthermore it is well known that thermal shrinkage of the separator or its mechanical rupture can lead to an abnormal heating, which may cause fire or explosion eventually. In this study we have developed a novel separator based on polymer/inorganic nanocomposite technology that can significantly improve battery safety. Basic properties of the ceramic-coated separator are investigated and its relationship with electrochemical performances in lithium-ion batteries is discussed. And finally, its contribution to the safety improvement is given.

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High Efficiency Organic Photovoltaic Solar Cells via Nano-Morphology Control of Photoactive Layers

조길원

포항공과대 화학공학과

고분자 유기태양전지의 효율 증대를 위해서는 새로운 광활성층의 합성과 아울러 광활성층의 나노 몰포로지 제어 및 계면구조의 제어가 중요하다. 이번 발표에서는 본 연구실에서 최근 몇 년 동안 수행된 계면구조 제어와 광활성층의 나노 몰포로지 제어에 대하여 소개한다.

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Developement of New Organic Semiconducting Materials for Lighting and Solar Cell

김윤희, *권순기

*경상대 화학과 *경상대 나노신소재공학부*

Soluble conjugated organic materials have received considerable attention because they can be processed in simpler and more cost-effective ways than their inorganic semiconductor counterparts. Their electronic and optical properties can be tuned via molecular design and synthesis. In semiconductors, the transport of holes and electrons are governed by the HOMO and LUMO energy levels. The energy levels of an organic semiconductor govern the efficiency of carrier injection and extraction, control the energy and electron transfer process at the heterojunction, and determine the intrinsic photophysical properties, such as absorption and emission. The opto-electronic properties of conjugated polymers can be effectively tuned by intramolecular charge transfer involving donor-acceptor interactions. The hybrization of HOMO located on the donor moiety with LUMO located on the acceptor moiety provides a means for tunning the electronic and optoelectronic properties in device applications, such as light emitting diodes, photovoltaic cells, field effect transistors, and memory devices. In this presentation, we report new organic semiconducting materials for lighting and solar cell through tunning the structure via molecular design and synthesis.

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Artificial Photosynthesis with water as both electron and oxygen atom donor

Inoue Haruo

Tokyo Metropolitan University

Artificial photosynthesis by visible light is one of the most desirable systems for human being to be realized. The possibility is, however, still questionable in spite of enormous efforts in the past, since the most important problem of how to utilize water molecule as an electron donor has not yet been solved. Recent efforts on photo-redox systems that can induce actual chemical reactions have focused much attention on the reduction terminal end of the photoredox systems rather than on the oxidation terminal end. Efficient hydrogen evolution1 and even carbon dioxide reduction have been reported. Only a very few reactions, however, can actually be coupled in the oxidative terminal end. Incorporation of a water molecule into the oxidative terminal end, i.e., oxidation of water as an ideal electron donor, should be one of the central subjects of study. Among various approaches for the oxidation of water, the oxidation of water should involve one of the following: 1) a one-electron process, 2) a two-electron one, or 3) a multi-electron one. The one-electron process, even the one-electron oxidation of the hydroxide ion, needs a rather high oxidation potential (>2.0 V), and the resultant hydroxide radical is too reactive to be handled. The multi-electron one, such as the four-electron process, requires a highly specific stereo-chemical arrangement, though the thermodynamic requirement for the process is milder. To avoid the difficulties of these two processes, among the actual photoreactions, we have recently focused our attention on the two-electron oxidation of water, which also has a mild thermodynamic requirement, sensitized by metalloporphyrins. Here, we report that a rutheniumII porphyrin as a sensitizer induces a highly selective epoxidation of alkenes with water both as an oxygen donor and a two-electron donor upon visible light irradiation. The highest quantum yields of the photochemical epoxidation turned out to be 0.60 for the formation of cyclohexeneoxide from cyclohexene, with a selectivity of 94.4 %, and 0.40 for norborneneoxide formation, with 99.7% selectivity. The reaction serves as one of the typical photoreactions that can incorporate a water molecule both as an oxygen atom donor and two-electron

donor. Recent progress in constructing the artificial photosynthetic system including CO2 reduction will be reported.

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Development of Artificial Photosynthetic Systems for Reduction of Water and CO_2

Won-Sik Han, Hyun-Young Kim, Chyongjin Pac, Sang Ook Kang

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The goal of artificial photosynthesis is to mimic the natural photosynthetic systems in the chemical conversion of solar energy. This still remains as a crucial and challenging issue in artificial photosynthesis due to difficulties in realizing up-hill conversion processes. Nonetheless, a number of promising approaches have appeared in recent years.

We had particular interest on visible-light-driven reduction of water and CO_2, and have explored the significance of hydrophilic and steric characteristics of organic dyes in sensitized H_2 generation based on Pt/TiO_2 catalysts. The optimization of hydrophilic character coupled with the minimization of steric effects is a key issue associated with the general guideline for designing organic dyes with high sensitization capability in H_2 generation. Also, photocatalytic CO_2 reduction using metal complexes, especially rhenium(I) complexes have been successfully achieved. This lecture will summarize recent advances of artificial photosynthesis related to the visible-light reduction of water and CO_2.

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Artificial Photosynthesis using Metal Complexes

Osamu Ishitani

Tokyo Institute of Technology

Both problems of the global warming and shortage of the fossil fuels have brought about great interest in artificial photosynthesis. In photosynthesis of green plants, electrons captured from water using solar energy are stored into the coenzyme NADP. The product NADPH is used for reduction of CO2 as a reductant in the Calvin cycle. Therefore, development of both photocatalysts for reduction of NADP and CO2, which require two-electron (hydride) reduction, should be important targets in the field of the artificial photosynthesis.I report our recent results about architectural investigation of such photocatalysts.We have developed highly efficient photocatalytic systems using the rhenium(I) complex(es) as either photocatalyst or catalyst for CO2 reduction.1 I will focus on the following systems in my talk.(1) Development of the most efficient photocatalystic system with two different Re(I) complexes (FCO = 59 %).1a(2) Architecture of supramolecular metal complexes with both Ru(II) and Re(I) complexes as photosensitizer and catalyst, respectively.2 Ordinary photocatalysts, which initiate intermolecular electron transfer, is useless for reduction of NADP model compounds to the corresponding 1,4-duhydroforms because of rapid coupling reactions of the one-electron reduced radicals of the models. (3) We have developed a novel type of photocatalytic systems which can drive only hydride reduction of an NADP model compound with high selectivity and efficiency.3 References1 (a) J. Am. Chem. Soc., 2008, 130, 2023-2031. (b) J. Am. Chem. Soc., 2005, 127, 15544-15555. (c) Res. Chem. Intermediat. 2007, 33, 37-48. (d) J. Photochem. Photobiol. A: Chem., 1996, 96, 171-174. (e) Organometallics, 1997, 16, 5724-5729. (f) J. Chem. Soc., Dalton Trans., 1997, 1019-1023.2 (a) Inorg. Chem., 2005, 44, 2326-2336. (b) Photochem. Photobiol. Sci., 2007, 6, 454-461. (c) J. Photochem. Photobiol., A: Chem. in press.3 (a) Inorganic Chemistry 2009, 48, 10138. (b) Chem. Eur. J. 2005, 11, 4219. (c)Organometallics 2001, 20, 3361. (d) J. Chem. Soc., Chem. Commun. 1994, 367.

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Thermally Rearranged Polymer Membranes Tuned to Capture CO2

이영무

한양대 화학공학

Thermally rearranged (TR) polymers with an intermediate cavity size, a narrow cavity size distribution and a shape reminiscent of bottlenecks connecting adjacent chambers yield both high permeability and high selectivity tuned for CO2 capture from flue gas. Our approach for intermediate sized cavities was to control free volume element formation.

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다상의 이산화탄소가 주입된 퇴적토의 지반공학적/지구물리학적 물성 파악

조계춘

KAIST 건설및환경공학과

온실가스 감축의무를 규정하는 교토의정서가 발효됨에 따라 우리나라는 이산화탄소 포집 및 저장 기술의 적극적인 활용을 통해 2020 년까지 연 250Mt-CO_2 감축을 목표로 한다. 우리나라의 경우는 대량의 이산화탄소를 육상에서 저장하는 것은 불가능하므로 대륙붕 등의 해저에 저장하는 해저 지중저장 방식이 필연적이다. 이를 위해 해저 지반내에 이산화탄소 하이드레이트를 이용해 인위적으로 불침투성 층을 형성하고 이 층 밑에 액체/초임계유체 상태의 이산화탄소를 주입하여 저장하는 이산화탄소 해저지중저장 방식의 가능성이 검토되고 있다. 본 연구에서는 이러한 저장방식에 대한 지반공학적 접근을 통해 이산화탄소가 주입된 지반의 안정성과 실현가능성에 대한 연구를 수행하였다. 이산화탄소의 주입률 및 주입량은 이산화탄소 지중저장의 경제성과 실효성을 결정짓는 중요한 요소이다. 따라서 본 연구에서는 실제 동해 울릉분지 퇴적토 지반 시료에 대한 유체상 이산화탄소의 주입률을 실험적으로 검증하였다. 한편, 이산화탄소 하이드레이트와 액상 이산화탄소를 포함하고 있는 지반의 거동과 그 안정성을 검증하기 위해서 역학적/수리학적 거동 모델을 개발하였다. 또한, 거동 모델의 검증을 위해서 실제 동해 울릉분지 퇴적토 지반시료 내에 다상 이산화탄소를 주입하고 탄성파 및 전기비저항 등의 비파괴탐사기법을 이용하여 그 포화도에 따른 지반공학적/지구물리학적 물성을 측정하였다. 본 연구를 통해 이산화탄소의 주입률과 지반의 토질 및 간극률간의 관계를 검증하였고 이산화탄소가 주입된 지반의 물성은 지반의 토질과 간극률, 유효응력과 함께 다상 이산화탄소의 포화도에 밀접한 상관관계를 보이고 있음을 확인하였다.

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Latest Progress in CO_2 Offshore Geological Storage

허철

한국해양연구원 해양안전방제기술연구부

Carbon dioxide Capture and Storage (CCS) is regarded as one of the most promising options to response severe climate change. CCS is to capture CO_2 from major point sources such as power plants and ironworks, to transport to the storage sites and to store CO_2 into the subsurface geological structure. Especially, offshore geological storage has been recognized as a more feasible method due to its reliability and practicality. Since 2005, we have developed relevant technologies and focused on the marine geological storage of CO_2. Those technologies include possible storage site surveys and basic designs for CO_2 transport and storage processes. To design a reliable CO_2 marine geological storage system, we devised a hypothetical scenario and used a numerical simulation tool to study its detailed processes. Before going to main calculation of process design, we compared and analyzed the relevant equation of states. Up to now, process design for this CO_2 marine geological storage has been carried out mainly on pure CO_2. Unfortunately the captured CO_2 mixture contains many impurities such as N_2, O_2, Ar, H_2O, SO_x, H_2S. A small amount of impurities can change the thermodynamic properties and then significantly affect the compression, purification and transport processes. Among them, non-condensable gases can make unexpected two-phase flow during the transport and injection process resulted in severe pressure drop, pulsation, etc. To predict the CO_2-N_2 mixture behavior, optimum binary parameter to consider the interaction of CO_2 and N_2 molecules was suggested based on the mean absolute percent error. And the existence of water in the CO_2 stream can make a hydrate during the high pressure and low temperature condition process. It is one of the most important design requirements to avoid the hydrate formation and predict hydrate behavior. The phase equilibrium of CO_2 gas mixtures, including water, hydrate and electrolyte, has been investigated. Two and three-phase equilibria were numerically simulated and experimentally verified. Dissolution behavior of CO_2 in water is also studies by analyzing the mass transfer of CO_2 into water through interfacial hydrate layer in convective conditions. The results of present studies will contribute to understanding not only how commercial-scale development and

deployment of CO_2 storage in marine geological structures can be feasible but also how more reliable and safe CCS could be achieved. The study also suggests that there may be a strong need for systematic and scientific research to ensure safe and secure storage of CO_2 in marine geological structures.

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Carbon dioxide absorption using ionic liquids

정민석, 김훈식

경희대 화학과

Among various new methods proposed for carbon dioxide absorption, a method using ionic liquid was studied intensively focusing on the advantages and disadvantages compared to current processes.

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Factors to be Considered in Applications of Metal-Organic Frameworks for Carbon Dioxide Capture

김자헌

숭실대 화학과

MOFs have been considered as promising gas storage or separating materials because of their large surface areas and controllable pore environments. However, other factors such as their process costs or water-stabilities must be considered before using these materials for practical applications. A full understanding is required for the specific chemical process of the MOF applications is required, and most academic researchers are incapable of carrying out this investigation. In this talk, these issues will be raised and discussed by relating the chemical and physical properties of selected MOFs to the practical CO2-capture processes.

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이산화탄소 포집 및 저장 기술의 개발 현황

김종남

에너지연구원

이산화탄소 포집 및 저장(CCS) 기술은 화력발전, 철강, 시멘트산업 등에서 대량으로 배출되는 CO2 를 고농도로 포집□압축□수송하여 지하의 염수층, 석탄층, 유정, 가스정 등에 안전하게 저장하는 기술이다. CCS 비용의 약 70%가 포집비용인데, 현재 석유화학산업에서 상업화 가동되고 있는 아민(MEA) 기반 CO2 흡수기술을 화력발전소에 적용하면 전기가격이 70% 이상 상승하므로 전세계적으로 대용량의 CO2 를 저비용으로 포집하는 기술이 개발되고 있다. CO2 수송과 저장은 기술수준이 상용화에 도달하여 세계적으로 CO2 를 저장소에 주입하고 거동을 예측하는 실증 위주로 진행되고 있다. G8, 국제에너지기구(IEA) 등은 2020 년 이후에 이산화탄소 포집 및 저장기술을 상용화 적용하겠다는 계획을 세우고 있으며, CCS 기술의 조기 상용화를 위하여 2020 년 이전에 전세계적으로 20 여기의 상용화 규모 CCS 시범사업을 할 것을 제안하고 있다. CO2 포집기술은 연소 후, 연소 전, 연소 중 기술로 분류된다. 400 MWe 이상의 배가스를 처리하는 CO2 포집기술을 개발하기 위하여 현재 20 MWe 급 암모니아수 흡수공정과 40 MWt 급 순산소 연소기술이 가장 앞서서 개발되고 있다. 그리고 연간 2 백만톤의 CO2 를 저장하는 실증설비가 가동 중이다. 여기서는 국내외의 기술개발 현황을 살펴보고, 앞으로의 기술개발 방향을 제시해 보았다.

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Outline of Research Activities in Korea Center for Artificial Photosynthesis

윤경병

서강대 화학과

The materialization and eventually the commercialization of artificial photosynthesis will be another big triumph of the mankind from the scientific, environmental, and economical points of view. The National Research Fund of Korea has recently launched a center called Korea Center for Artificial Photosynthesis (KCAP) in Sogang University on Sep 30, 2009. In this center various research and development activities aimed to materialize artificial photosynthesis in the laboratory scale and eventually to develop commercially viable artificial photosynthesis processes are being conducted. The outline of the on-going activities of KCAP and its recent achievements will be presented.

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Ice and Like-Ice: Challengeable and Mysterious Material

이혼

KAIST 생명화학공학과

Ice appears in nature in forms as varied as snowflakes and hail, icicles, glaciers, pack ice, and entire polar ice caps. It is an important component of the global climate, particularly in regard to the water cycle. Furthermore, ice has numerous cultural applications, from the ice cooling one's drink to winter sports and ice sculpture. Called methane hydrate, or gas hydrate, it's an ice-like substance composed of methane, the main constituent of natural gas, trapped inside cages of water molecules. It forms under pressure, with deposits found underneath permafrost in Arctic regions and beneath deep ocean floors. But flammable ice is a fair description of the planet's most abundant, if least recognized, form of fossil energy. At moderate temperature and pressure conditions small guest molecules are entrapped in pure ice powders to form the mixed icy hydrate materials, followed by ion inclusion in confined empty ice-cages. For the complete accomplishment of anion transfer the ions or electrons are migrated through ice lattice, establishing the powerful and highly efficient ionic transport. First of all, the pure ice is transformed to the ionized ice by imprisoning ionic species into the confined space of icy cages. As the first attempt we synthesize the ionic icy materials (IIM) containing energy gases such as H_2 and CH_4. The formed IIMs are recommended to exhibit high ionic conductivity comparable to Nafion, a commercial electrolyte, and high capacity for storing energy gases. A variety of ionic icy materials will be tested until we find the best one with amazing performance. The unique behavior of IIM is deeply examined to prove its promising application to highly sensitive energy devices. For the first time we attempt to establish energy storage and production systems as icy nano-reactors in which the active reactions between active ice lattice and active guest molecules or between active guest molecules can take place. More significantly, the novel design and synthesis of reactive icy hydrates are expected to open a new field for inclusion chemistry and ice-based science and technology. The return after success might be quite surprising and unimaginable. The energy-related breakthrough technologies will significantly overcome the critical limitations of the existing future energy approaches.

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발표분야: 이산화탄소 분리, 저장 및 자원화 II
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이산화탄소 지중 저장의 효율성 및 안정성에 대한 광물학적 조성의 영향 평가를 위한 다상 열-수리-화학적 수치 모델링

김준모

서울대 지구환경과학부

본 연구에서는 국내 이산화탄소 지중 저장 유망 대상 지층 중의 하나인 경상분지 신동층군 하산동층 내의 이산화탄소 지중 저장에 의한 지하수와 이산화탄소 유동 및 반응성 용질 이동을 통합적으로 분석하고, 지중 주입된 이산화탄소의 수리동역학적 포획, 용해 포획 및 광물 포획 기작의 효율성 및 안정성에 대한 대상 지층의 광물학적 특성과 조성 변화(녹니석의 체적 분률 = 0.00%, 3.00%, 6.93%, 9.00%)의 영향을 정량적으로 평가하기 위하여 일련의 다상 열-수리-화학적 수치 모델링을 수행하였다. 수치 모델링 결과들은 지중 주입된 이산화탄소가 자유 유체상의 형태로 부력에 의해 먼저 상부로 이동하여 저장암과 덮개암의 경계면을 따라서 이산화탄소의 구조 포획 및 잔류 포획이 일어나고, 그런 다음에 자유 유체상의 이산화탄소가 차지한 영역을 중심으로 이산화탄소의 용해 포획이 발생하며, 마지막으로 이산화탄소의 용해 포획에 의해 지하수의 pH 가 낮아진 영역을 중심으로 다양한 지하수와 광물 간의 화학 반응을 통하여 이산화탄소의 광물 포획이 진행됨을 보여준다. 먼저 모든 경우에서 지하수의 pH 가 낮아진 영역을 중심으로 저장암을 구성하는 일차 광물 중에서 정장석, 사장석 및 녹니석은 용해되며, 석영과 일라이트는 침전된다. 한편 일차 광물 중에서 방해석은 이산화탄소 지중 주입 초기에 pH 가 낮아진 영역을 중심으로 용해되다가 시간이 지남에 따라서 외부 영역에서 다시 침전되며, 녹니석의 체적 분률이 0.00%인 경우에는 지속적으로 침전되고 그 외의 경우에는 점차적으로 이차 탄산염 광물인 도소나이트, 능철석, 앵커라이트 및 마그네사이트로 전환된다. 또한 일차 광물 중에서 적철석은 pH 가 낮아진 영역에서 용해되며, 시간이 지남에 따라서 pH 의 중성-염기성의 경계부에서 침전된다. Na-스멕타이트, Ca-스멕타이트 및 카올리나이트 등의 이차 광물들은 시간이 지남에 따라서 침전된다. 한편 이산화탄소의 광물 포획은 녹니석의 체적 분률이

0.00%인 경우에는 주로 도소나이트와 방해석의 침전을 통해서, 그 외의 경우에는 주로 능철석, 앵커라이트 및 마그네사이트의 침전을 통해서 이루어진다. 능철석은 초기에는 침전되지만 시간이 지남에 따라서 앵커라이트로 전환된다. 그리고 모든 경우에서 이차 광물로 고려된 백운석과 황철석은 침전되지 않는다. 이산화탄소의 광물 포획에 대한 기여도는 앵커라이트가 가장 높다. 또한 이산화탄소의 광물 포획에 기여하는 이차 탄산염 광물들(능철석, 앵커라이트 및 마그네사이트)의 침전에 필요한 Mg^{2+}와 Fe^{2+}는 주로 녹니석의 용해에 의해서 공급된다. 따라서 대상 지층의 광물학적 조성 변화에 따른 이산화탄소의 광물 포획의 효율성과 안정성은 녹니석의 함량에 가장 민감하며, 녹니석의 함량이 증가할수록 이산화탄소의 광물 포획의 효율성과 안정성이 증가한다. 사사 : 본 연구는 환경부 산하 한국환경산업기술원의 토양·지하수오염방지기술개발사업 연구비 지원에 의해 수행되었습니다.

대한화학회 THE KOREAN CHEMICAL SOCIETY

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장소: 송도컨벤시아
발표코드: **금6E7심**
발표분야: 이산화탄소 분리, 저장 및 자원화 II
발표종류: 심포지엄, 발표일시: 금 16:40, 좌장: 최원용

Adsorption and Desorption of CO_2 and CH_4 on Korean Coal under Subcritical to Supercritical Conditions

Chang-Ha Lee

Department of Chemical and Biomolecular Engineering, Yonsei University, Seoul, Korea

Coal seams have been reported as possible storage sites for CO_2 to help mediate the global greenhouse gas problem. In addition, enhance coal bed methane (ECBM) using compressed CO_2 has been attracted due to the production of clean energy and CO_2 storage. The adsorption and desorption characteristics of CO_2 and CH_4 on dry and wet Korean coal (Kyungdong, anthracite coal) were studied using a static volumetric method at 298, 318 and 338 K, and up to 150 atm. The adsorption of CO_2 and CH_4 was favorable at low temperature and dry coal conditions. The hysteresis of coal swelling through adsorption, desorption and readsorption of CO_2 was observed at subcritical condition. Hysteresis between adsorption and desorption isotherms occurred in both dry and wet coals. The crossover between adsorption and desorption isotherms in dry coal was observed near the critical region, while the excess amount of adsorbed CO_2 on wet coal was lower during desorption than during adsorption. However, the crossover was not observed in CH_4 adsorption on coal and hysteresis was relatively small. Structural variations of the coal after the wet experiment were significant compared to those in the dry coal. In wet coal, the dissolution of H_2O in the CO_2 or CH_4 phases, absorption of CO_2 or CH_4 in the aqueous phase, and coal structure changes affected the estimation of adsorption amount, especially under supercritical condition.

Keywords: carbon dioxide; methane; coal; high-pressure adsorption; coal swelling

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장소: 송도컨벤시아

발표코드: **목7I1분념**

발표분야: 생체내 화학에서의 금속

발표종류: 분과기념강연, 발표일시: 목 13:30, 좌장: 김진홍

[우수연구상수상기념강연] Metal Oxides are Magic: from Superconductors to Catalysts

허남회

서강대 화학과

Metal oxides are technologically important materials that have a wide range of applications. Their properties largely depend on the nature of transition metals and their structures. For example, copper oxides with layered structure show superconductivity while colossal magneto resistance is observed only in perovskite manganese oxides. Among these applications, the use of metal oxides as catalysts is the most important issue in the chemical society. They are the functional components in the catalysts used in a large number of selective oxidation processes. Recent advances in metal oxide chemistry will briefly be reviewed in this talk. In addition, the emphasis will be on the synthesis and catalytic properties of Au, Rh, and Pt nanoparticles immobilized on a superparamagnetic mesoporous silica microsphere, denoted as M-CoFe2O4@SiO2 (M = Au, Rh, Pt).

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발표분야: 생체내 화학에서의 금속
발표종류: 심포지엄, 발표일시: 목 14:20, 좌장: 조재흥

The Development of New Heme-Copper and Heme Nitrogen-Oxide and Dioxygen Chemistry

Kenneth D. Karlin

Department of Bioinspired Science, Ewha Womans University, Seoul, KOREA and The Department of Chemistry, Johns Hopkins University, Baltimore, MD, USA

Our ongoing interests in copper/dioxygen and heme/copper/dioxygen bioinorganic chemistry have led us to probe new chemistries that include nitrogen monoxide (·NO), a radical diatomic molecule with a history in transition metal chemistry and importance in biology and metallo-enzymology. Here, we describe nitrogen monoxide reductive coupling chemistry, a reactions carried out by denitrifying bacteria, but which is also effected by heme-copper oxidases such as cytochrome *c* oxidase. It is the latter chemistry which we have been able to show which can take place. Heme-copper assemblies can also produce nitrogen monoxide via nitrite reduction chemistry and preliminary results on that chemistry will be discussed. We also demonstrate the likely generation of a peroxynitrite-heme moiety ($O{=}N{-}O{-}O^-$; normally described as the product of superoxide anion plus ·NO) derived from a heme-dioxygen adduct which reacts with nitrogen monoxide to give a heme-nitrate final product.

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발표분야: 생체내 화학에서의 금속
발표종류: 심포지엄, 발표일시: 목 14:50, 좌장: 조재흥

Efficient Catalytic Systems for Hydrogen Production and Storage

Shunichi Fukuzumi

Department of Material and Life Science, Osaka University, Suita, Osaka, Japan & Department of Bioinspired Science, Ewha Womans University, Korea

Hydrogen is a clean energy source for future and focused attention on alternative energy to fossil fuel because the reaction of hydrogen with oxygen produces the requested energy and only water as an environmentally-friendly side product. However, the storage and transfer of hydrogen are difficult with current technology, since hydrogen gas is explosive and has a poor energy density. The interconversion of H_2 with CO_2 to formic acid (HCOOH) (eq 1) in the presence of an appropriate catalyst merits special attention.[1]

$$H_2 + CO_2 \rightleftharpoons HCOOH \quad (1)$$

This lecture focuses on efficient catalytic systems for CO_2 fixation with H_2 to form HCOOH and the selective decomposition of HCOOH to H_2 and CO_2,[2,3] as well as efficient photocatalytic systems for hydrogen production.[1,4]

(1) Fukuzumi, S. *Eur. J. Inorg. Chem*. **2008**, 1351.

(2) Fukuzumi, S.; Kobayashi, T.; Suenobu, T. *ChemSusChem* **2008**, *1*, 827.

(3) Fukuzumi, S.; Kobayashi, T.; Suenobu, T. *J. Am. Chem. Soc*. **2010**, *132*, 1496.

(4) Fukuzumi, S. *Phys. Chem. Chem. Phys*. **2008**, *10*, 2283.

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발표코드: **목7I3심**
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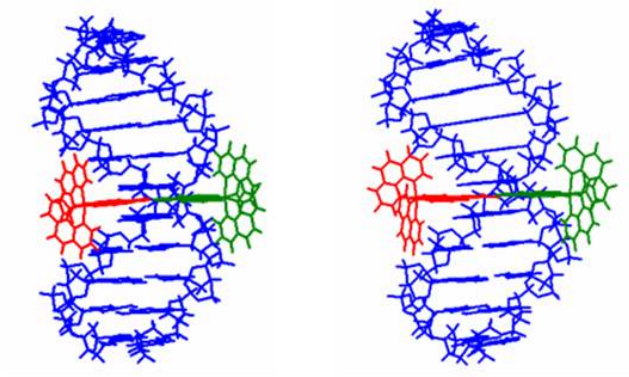
발표종류: 심포지엄, 발표일시: 목 15:30, 좌장: 이용민

Interaction of various Ru(II) complexes with single- and double-stranded DNA

김석규

영남대 화학과

Interaction between the metal complexes containing planar aromatic ligands and various DNAs have been widely studied. A representative metal complex in this group is octahedral ruthenium complexes such as $[Ru(phen)_2L]^{2+}$, which have been investigated as probes of nucleic acid structure, as chemical nuclease, as fluorescence probes and in electron transfer system. In the symposium, various physical aspect of Ru(II) complex upon binding to DNA will be discussed. When 4',6-diamidino-2-phenylindole (DAPI), which has been known to bind at the AT rich-region of double stranded DNA, and Ru(II) complex were simultaneously bind to DNA, the luminescence intensity of DAPI decreased while that of the Ru(II) complex increased, indicating that the Ru(II) complex acted as a donor in the through DNA energy transfer system. It was recently found that the luminescence intensity of the Ru(II) complex increased upon binding to the single-stranded DNA. This observation suggested that the DNA stranded can surround the Ru(II) complex thereby protecting the water molecule resulting in a "light switch effect". In addition to these two physical aspect of the Ru(II) complex, the binding mode of various *bis*-Ru(II) complex to DNA will be discussed.



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발표코드: **목7I4심**
발표분야: 생체내 화학에서의 금속
발표종류: 심포지엄, 발표일시: 목 16:00, 좌장: 이용민

Efficient Olefin Epoxidation by Non-Heme Mn(III) Complexes with Peracids: Evidence of the Multiple Active Oxidants, Mn(V)=O, Mn(IV)=O, and Mn(III)-OO(O)CR Species

김철

서울산업대 정밀화학과 친환경소재제품센터

Two new tetranuclear chalcocyanide cluster complexes, [{Mn(saloph)H2O}4Re4Q4(CN)12]•4CH3OH•8H2O (saloph = N,N'-o-phenylenebis(salicylidenaminato), Q = Se (1-Se), Te (2-Te)), and two mononuclear nonheme Mn(III) complexes of tetradentate ligands containing two deprotonated amide moieties, [Mn(Me_2bpb)Cl(H_2O)] (3) and [Mn(bpc)Cl(H_2O)] (4), were prepared and characterized by IR and elemental analysis. Complexes 2-Te and 3 have also been characterized by X-ray crystallography. These complexes catalyzed efficiently a wide range of olefin epoxidation upon treatment with meta-chloroperbenzoic acid (MCPBA), under mild experimental conditions. Olefin epoxidation by these catalysts was proposed to involve the multiple active oxidants Mn(V)=O, Mn(IV)=O, and Mn(III)-OO(O)CR. Evidence for this approach was derived from reactivity and Hammett studies, $H_2{}^{18}O$-exchange experiments, and the use of peroxyphenylacetic acid as a mechanistic probe. Moreover, it has been observed that the participation of Mn(V)=O, Mn(IV)=O, and Mn(III)-OOR can be controlled by changing the substrate concentration. This mechanism provides the greatest congruity with related oxidation reactions by using certain Mn complexes as catalysts.

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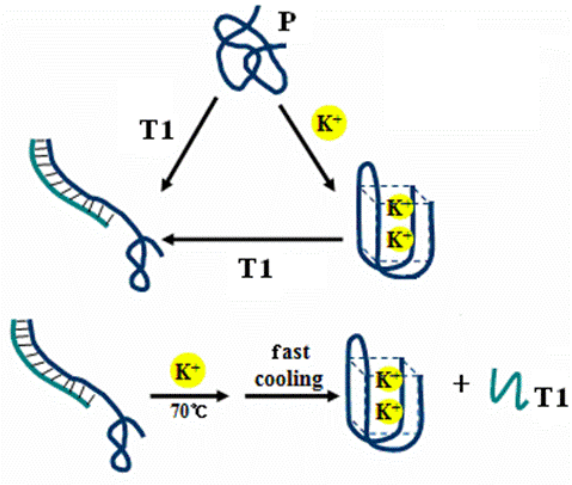
발표종류: 심포지엄, 발표일시: 목 16:30, 좌장: 이용민

Sensitive and Selective Detection of Adenosine and Potassium Ions Using Oligonucleotide-based Probes

김진홍

이화여대 화학과

Recently, sensing of small molecules and ions coupling the attractive properties of aptamers has received considerable attention. Electrochemistry offers attarctive routes for interfacing aptamer interactions with the signal generating element in a simple, fast, and inexpensive manner. Modern electronic aptamer biosensors commonly rely on redox tags with conformational changes, or impedance detection to offer convenient measurements of nanomolar concentrations of target molecules. Further enhancement of the sensitivity of such devices is urgently needed for measuring ultra low levels of target agents. Recent studies to improve the sensitivity of aptamer-based biosensors and bioassays have lowered their detection limits to the picomolar level through the use of nanoparticle tags, binding-induced conformational changes, and label-free impedance detection. We herein present an electrochemical and fluorescence assay of adenosine and potassium ions based on aptamer-based sensors with metal complexes utilizing a specific interaction between DNA and metal complex.



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발표분야: 생체내 화학에서의 금속
발표종류: 심포지엄, 발표일시: 목 17:00, 좌장: 이용민

Catalysts for Water Oxidation and their Appllication in the PhotoElectroChemical(PEC) Cell

윤성호

국민대 생명나노화학과

In the future, fuel cells, using solar energy for the generation of renewable energy such as hydrogen and methanol, are appealing systems in the point of the decreasing energy sources and the environmental problems arising from combustion of oil and gas in air. A promising approach to eventual utilization of solar energy is to mimic natural photosynthesis in green plants, which use electrons from water oxidation to reduce carbon dioxide into "fuel"Photosynthesis in green plants uses the conjugated process of water oxidation into molecular dioxygen and simultaneous reduction of carbon dioxide into carbohydrate. Photosystem II is a key enzyme in this process, utilizing two conjugated machineries so called photosensitizer and oxygen evolving center (OEC). We have recently developed a unique bioinorganic approach to mimicking the function of oxygen evolving center, and have used the gain lessons to fabricate photoelectrochemical(PEC) cells. The results of this investigation will be presentedAcknowledgement: This work was supported by the Korea Science and Engineering Foundation(KOSEF) grant (NO. R01-2008-000-11812-0) funded by the Korea government(MEST)

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발표분야: 무기화합물의 융합화학
발표종류: 심포지엄, 발표일시: 금 09:30, 좌장: 이광렬

[3+2] Cycloaddition of Azides Alkyne-Azide in Various CuO Hollow Nanospheres

박강현

부산대 화학과

CuO hollow nanospheres and CuO hollow nanospheres on acetylene black (CuO/AB), were synthesized and used for the catalytic [3+2] cycloaddition of azides with terminal alkynes to provide products in good yields with high regioselectivity. In addition, CuO/AB have been used for the catalytic [3+2] cycloaddition of azides with terminal alkynes without solvent, and within one minute under microwave irradiation. The CuO/AB was readily separated by centrifugation, and could be reused five times under the present reaction conditions without any loss of catalytic activity.

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발표분야: 무기화합물의 융합화학
발표종류: 심포지엄, 발표일시: 금 10:00, 좌장: 이광렬

Site isolations of catalytically active Mn-porphyrin via supramolecular encapsulation and nanoscopic immobilization

이석중

고려대 화학과

Transition metal meditated coordinative self-assembly has shown tremendous growth over the past decade. Many assemblies have not only shown interesting structures but also demonstrated applications in catalysis, chemical sensing, and selective inclusion of guest molecules. Previously, it has been demonstrated the encapsulation of a manganese porphyrin catalyst within a large porphyrin-derived cavity structure, and a post-synthetic approach to improve both reaction stability and selectivity via supramolecular complexation. However, several factors limited the success of this post-synthetic supramolecular encapsulation system. These are: a) ligand binding on the outside of, rather than within, the cavity and b) rotational freedom of the cavity walls and the encapsulated catalyst. I envision that properly designed porphyrin building blocks will allow the formation of supramolecular boxes containing rigid porphyrin side walls with functionalisable cavities to overcome these limitations. In this talk, I wish to describe the assembly of pyridine containing porphyrin dimers which interact with linear zinc porphyrin trimers to construct porphyrin boxes via self-sorting processes. I will also talk about the site isolation of Mn-porphyrin via deposition on magnetic nanoparticles to prevent self-degradation process during the oxidation reaction.

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발표분야: 무기화합물의 융합화학
발표종류: 심포지엄, 발표일시: 금 10:30, 좌장: 이광렬

Novel magnetization mechanism for highly magnetic core-shell nanoparticles

윤태종

차의과학대 바이오산업응용학과

Magnetic nanoparticles (MNPs) with high magnetic moments and very small size are under active development as such materials find growing uses in biotechnology and medicine. Ferromagnetic metals rather than their corresponding oxides, have been suggested as an ideal constituent for MNPs. Unfortunately, monometallic MNPs typically require protective layers to prevent progressive oxidation, which often results in reduced overall magnetization. Here we present a new monometallic MNP consisting of an elemental iron core and an artificial ferrite-shell. The iron cores were enlarged into a thermally stable ferromagnetic state. Subsequently, protective ferrite shells were grown onto the cores and metal-doped to further enhance magnetization. The resultant particles displayed a unique magnetic feature, the presence of hysteresis with negligible coercivity. Further analysis revealed that the shell effectively reduces the coercivity of ferromagnetic cores by leading the magnetization process at small magnetic fields. The MNPs had very high magnetization and transverse relaxivities, and could be used for highly sensitive detection of proteins in the pico-molar ranges and single cancer cells. The mechanism and MNP featured here could serve as a new strategy in preparing stable, highly magnetic and yet dispersible nanoparticles from ferromagnetic crystals.

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발표분야: 무기화합물의 융합화학
발표종류: 심포지엄, 발표일시: 금 11:10, 좌장: 정옥상

Si-base Materials for Organic-Inorganic Hybrids

유복렬

KIST 나노재료센터

In recent years, much attention has been paid to organic-inorganic hybrid materials applicable to automotive, display device, fuel cell membrane, architecture, biocompatible materials, environment applications, and etc. The hybrid materials formed by the combination of inorganic materials and organic polymers are attractive for the purpose of creating high-performance or high-functional composite materials. Of particular interest is the nano-size level combination of two different components that may lead to new composite materials, termed 'organic—inorganic hybrid materials'. Recently, we have studied Si-based materials for organic-inorganic hybrids, especially the modification of nanosilica using organosilanepolyol and its characterization, composition with synthetic rubber. Some improvements of the properties these materials have also been explored from the viewpoint of industrial applications. In the symposium, I will present the synthesis and applications of Si-based materials for organic-inorganic hybrids in details.

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발표종류: 심포지엄, 발표일시: 금 11:40, 좌장: 정옥상

Triarylborane-based Lewis Acids for the Selective Complexation of Anions

이민형, *박명환, 김태원, *도영규

*울산대 화학과 *KAIST 화학과*

The detection of anions such as fluoride and cyanide ion is recently of great interest owing to high toxicity in physiological systems, as well as environmental concerns raised by widespread uses of such anions. Recently, triarylborane-based receptors have attracted great attention due to their high Lewis acidity. To search for a highly selective sensor system, we have introduced new concepts in designing novel triarylboranes such as cationic mono- and bidentate boranes, energy transfer system, polymeric borane, and *o*-carborane-borane dyads. In the cationic boranes, it was revealed that the fluoride affinity of boron centers in the phosphonium and ammonium boranes can be enhanced by favorable Coulombic attraction. Secondly, we designed a discrete and highly fluorescent borane-based sensor that exploits intramolecular excitation energy transfer transitions for the selective detection of cyanide by combining three-coordinate borane as an energy donor and highly fluorescent BODIPY as an acceptor. Thirdly, the synthesis of well-defined polymeric boranes was achieved via the direct copolymerization of ethylene and triarylborane-substituted 1-olefin monomer. The use of group 4 catalyst efficiently afforded triarylborane-functionalized polyethylene that is stable in ambient air conditions. Finally, we found that the introduction of an *o*-carborane cage into the triarylborane significantly enhances the Lewis acidity of the boron atom leading to large increase in fluoride ion affinity. Details of synthesis, structures, and the anion binding properties of triarylboranes will be presented.

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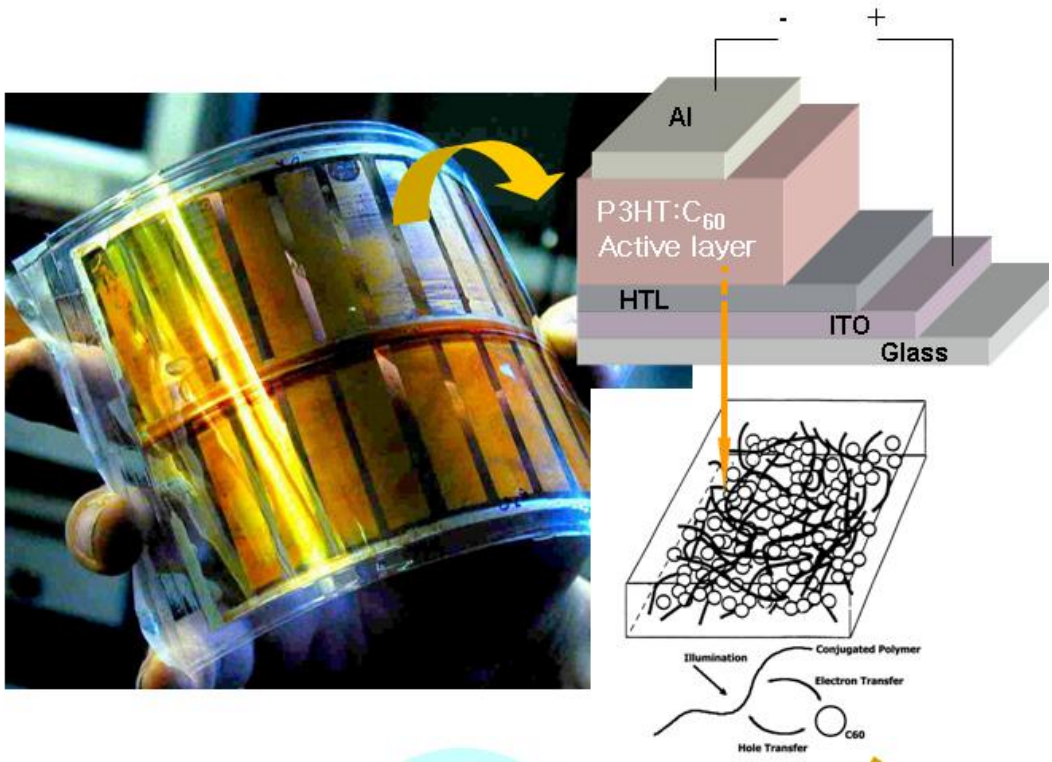
Ultrafast dynamics of photo-generated mobile carriers in polymer:fullerene bulkheterojunction solar cells

황인욱, 이창렬

광주과학기술원 고등광기술연구소

The bulk heterojunction (BHJ) material comprised of semiconducting polymer and the soluble fullerene derivative, PCBM, has exhibited high solar-to-electric power conversion efficiency in polymer-based solar cells. We have investigated the generation mechanism of mobile carriers and the carrier recombination/decay dynamics underlying the high performance of this system. We find that in polymer:fullerene composites mobile carriers are generated via a two step process: An initial ultrafast electron transfer to a charge transfer (CT) bound state, followed by the injection of mobile carriers into the bicontinuous network. We show that the carrier recombination is affected by the time spent in the CT bound state. Our ultrafast spectroscopic studies unravel the interplay between these processes (which determine the eventual photovoltaic device performance) and their dependence on the specific electronic structure in the crystalline and amorphous regions within the nano-structure of the polymer composite.


-
+
Al
P3HT:C60
Active layer
HTL
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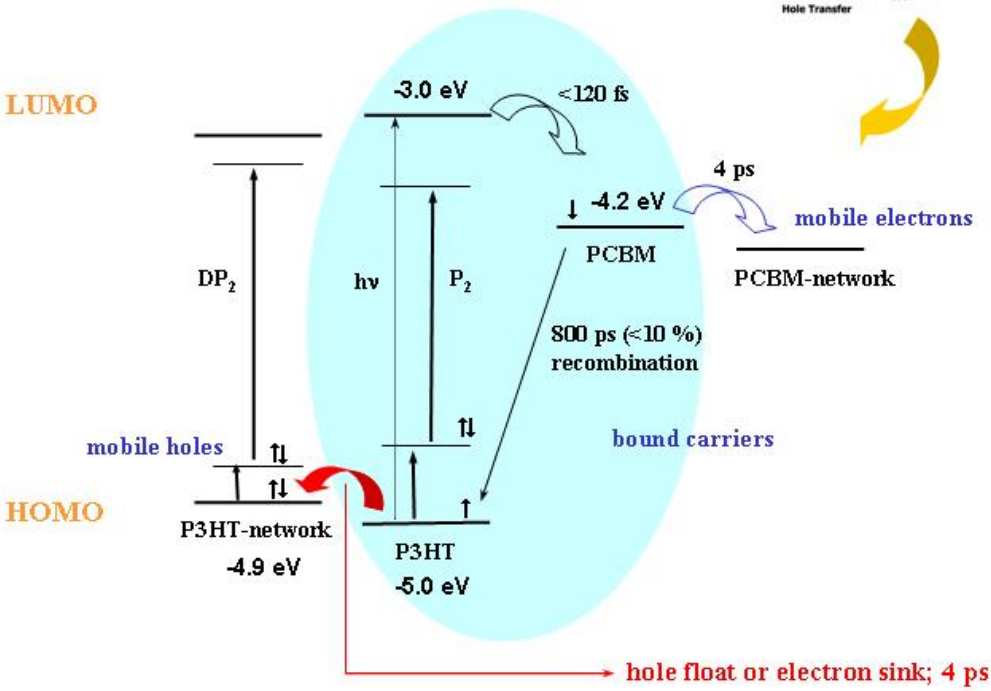
Glass

Illumination
Conjugated Polymer
Electron Transfer
C60
Hole Transfer


LUMO
-3.0 eV
<120 fs
4 ps
-4.2 eV
mobile electrons
PCBM
PCBM-network
DP2
hν
P2
800 ps (<10 %)
recombination
bound carriers
mobile holes
HOMO
P3HT-network
-4.9 eV
P3HT
-5.0 eV
hole float or electron sink; 4 ps

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발표종류: 심포지엄, 발표일시: 금 09:35, 좌장: 이남기

Charge-Transfer Enhancement in the Single-Molecule SERS

김지환

고려대 화학과

We measured the surface-enhanced Raman scattering (SERS) of individual gold nanoparticle - aminobenzenethiol (ABT) monolayer - gold film junctions to investigate the charge-transfer (CT) enhancement of SERS signals. Despite mild electromagnetic field enhancement (~10^5) and high surface density of ABT-molecules (~200 molecules / hotspot) at the junctions, we observe clear spectral and temporal signatures of CT-assisted single-molecule SERS (SM- SERS). The results demonstrate that only a small fraction of molecules at the junction site have significant CT-enhancement of ~10^2, whereas the rest of the molecules are nearly CT-inactive. Furthermore, the results also show that overall (charge-transfer and electromagnetic) enhancement of ~10^7 is sufficient to observe the SM-SERS of a non-resonant molecule, which starkly contradicts wide-spread belief on the minimum enhancement of ~10^{14} for SM- SERS.

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발표종류: 심포지엄, 발표일시: 금 10:00, 좌장: 이남기

Direct Observation of β-carotene's excited states by femtosecond stimulated Raman in the resonance domain

심상덕

삼성전기(주) 중앙연구소 분석그룹

Ultrafast vibrational spectroscopy is ideally suited to explore the excited-state structure of molecules involved in photochemistry due to the inherently high spectral resolution and sensitivity to molecular structure. However, time-resolved vibrational techniques have conventionally been limited to the picosecond time domain, making the direct observation of structural changes related to chemical reaction very elusive. To address this challenge, we have been developing the technique of time-resolved femtosecond stimulated Raman spectroscopy (FSRS), which provides vibrational spectra with high time (

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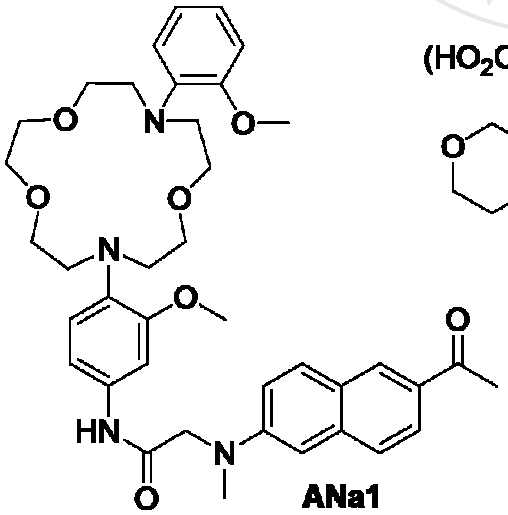
발표종류: 심포지엄, 발표일시: 금 10:45, 좌장: 성봉준

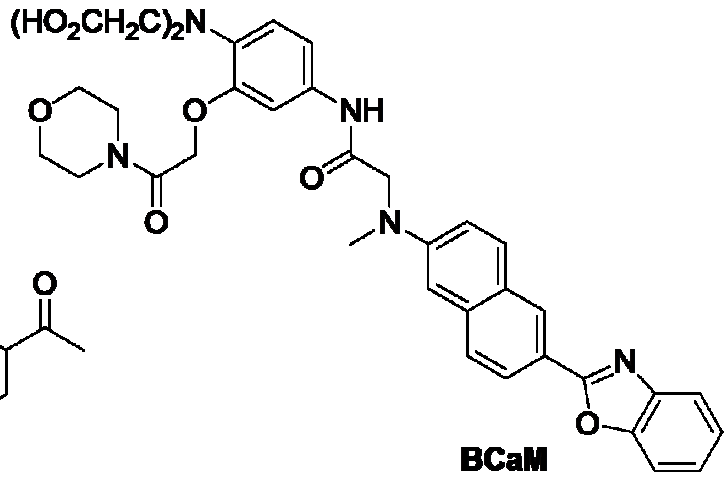
Two-Photon Fluorescent Probes for Na^+/Ca^{2+} Activities in Vivo

김환명

아주대 에너지시스템학부

Two-photon microscopy (TPM), which utilizes two near-infrared photons of lower energy for the excitation, has emerged as an indispensable tool in biology due to the capability of imaging the intact tissue for a long period of time with minimum interference from the tissue preparation artifacts, self-absorption, auto-fluorescence, photobleaching, and photodamage. To make it a versatile tool in biology, a variety of two photon probes for specific applications are needed.Herein, we report ANa1 and BCaM, which are capable of detecting the cytosolic free Na^+ ions and the near plasma membrane Ca^{2+} ions, respectively, and can simultaneous dual-color imaging the activities of Na^+/Ca^{2+} in live cells and tissues at >100 μm depth for a long period of time.





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Enhanced light harvesting in semiconductor photocatalysis

박현웅

경북대 물리 및 에너지학부

Semiconductor photocatalysis has received great attention over the past decades. The key issue to be addressed in the field is how to maximize the light conversion efficiency. Various attempts have been made to achieve this goal such as nano-sized metal loading on the semiconductor surface, (non)metal-doping into the semiconductor lattice, introduction of inorganic ions, surface charge modification, semiconductor-semiconductor binary systems, dye-sensitization, etc. This presentation will summarize briefly the aforementioned modification studies and then discuss the recent results regarding mesoporous titania nanofiber and semiconductor-carbon nanotube hybrids.

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in vitro light-harvesting antenna supercomplexes reveal plant photoprotection

안태규

성균관대 에너지과학과

In plants, antenna supercomplexes (SCs) play two opposing roles; efficiently transfering absorbed energy to reaction center (photosynthesis) and harmlessly dissipating excessively absorbed light energy as heat (photoprotection).(1) The former is to generate sugars and chemical energies for plant survival, instead the latter aims to avoid inevitably generated deleterious oxygen-related byproducts (i.e. reactive oxygen species). The radiation-less relaxation is called non-photochemical quenching (NPQ) and is critical for plant survival and fitness.(2) NPQ is predominantly mediated by a rapid response to photon flux density, or energy-dependent quenching (qE). qE can regulate reversibly photosynthesis depending on low lumen pH, de-epoxidized xanthophylls, e.g. zeaxanthin (Z), and the antenna-associated membrane protein PsbS. All these components of qE are linearly correlated to charge transfer (CT) quenching involving an electron transfer from Z to chlorophyll(s) (Chls) in thylakoid membranes of C-3 plant Arabidopsis thaliana.(3-5) Antenna SCs in photosystem II (PSII) are composed of LHCII trimers, major peripheral antenna light-harvesting complexes (LHCs), and minor chlorophyll protein complexes (mCPs, i.e. CP24, CP26, and CP29). All the LHCs contain chlorophylls (Chls) a and b, and carotenoids (Cars), i.e. lutein (L), violaxanthin (V), and neoxanthin (N). In light-adapted plants, specifically V can be converted into Z by an enzyme i.e. violaxanthin de-epoxidase which is activated under low pH. To pinpoint where CT quenching occurs in antenna SCs, we explored antenna LHCs systematically from LHCII trimer to individual LHC monomers; each comparing with Z-bound and V-bound LHCs which are analogs to light-adapted and dark-adapted conditions, respectively. Recently we found CT quenching in all isolated mCPs (CP24, CP26, and CP29),(4, 6, 7) while we could not observe any trace of Z•+ in LHCII trimer.(4) Furthermore, especially in CP29 we revealed molecular architecture of CT quenching including a Chl dimer (Chls A5 and B5) and Z.(6) mCPs are proximately located in the middle between LHCII antenna

and D1/D2 core complexes where the reaction centers (RCs) are located, a perfect geometry to regulate the downstream energy flow from antenna LHCs to RCs.

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2. Kulheim, C et al. Science 2002, 297, (5578), 91-93.

3. Ahn, T. K. et al. Chem. Phys. 2009.

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6. Ahn, T. K.et al. Science 2008, 320, (5877), 794-797.

7. Avenson, T. J. et al. J. Biol. Chem. 2009.

대 한 화 학 회
THE KOREAN CHEMICAL SOCIETY

일시: 2010년 4월 29~30일(목~금) 2일간
장소: 송도컨벤시아
발표코드: **목10A1분념**
발표분야: 분자구조 및 화학반응동력학:물리화학자의 관점
발표종류: 분과기념강연, 발표일시: 목 14:00, 좌장: 이진용

[입재물리화학상수상기념강연] A Story of Proline for Two Decades

강영기

충북대 화학과

The proline (Pro) residue is unique because the side chain is bonded to the amide nitrogen and the N-C rotation is restrained at about -60°. The prolyl five-membered ring may adopt two distinct puckered conformations, both frequently encountered in X-ray structures of peptides and proteins. The peptide bond is known to dominantly prefer the trans conformation in proteins. Analyses of X-ray protein structures show that the cis populations are ~6% for the prolyl peptide bond and ~0.04% for the nonprolyl peptide bond. It has been reported that the cis-trans isomerization of the X-Pro bond is often involved in the rate-determining steps for folding and refolding of various proteins. In addition, the prolyl cis-trans isomerization was reported to serve as molecular switches or timers in several biological systems. In this talk, I will focus on why proline has been interested and what known for proline by previous quantum-chemical studies. In addition, the ongoing works explored by recently developed density functionals with dispersion corrections and their applicability to the conformational study of bioactive peptides will be addressed.

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발표종류: 심포지엄, 발표일시: 목 14:30, 좌장: 최명룡

Cluster ions with hydrogen bond networks: structure, dynamics, and control

박승민

경희대 이과대학 화학과

Photodissociation dynamics of cluster ions with hydrogen bond network has been investigated. The kinetic energy releases of water molecules were measured at spectral ranges from IR to UV to shed light on the dynamics of energy transfer through hydrogen bond network. The average number of ejected water molecules measured as a function of photon energy over a wide range from visible to UV revealed that the loss of water molecules is certainly a stepwise photoevaporation process. The structural changes in the hydrogen bond networks were examined via IR photodissociation of the cluster ions. Also, “mode-aided” predissociation of water molecules in ternary ions with different solvent molecules has been attempted in their IR photodissociation.

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발표종류: 심포지엄, 발표일시: 목 14:55, 좌장: 최명룡

REMPI and IR-UV double resonance spectroscopy of 3-aminophenol•ammonia cluster

강혁

아주대 화학과

The near-UV exited state dynamics of phenol and solvated phenol in the gas phase is characterized by excited state hydrogen transfer (ESHT) reaction on a $^1\pi\sigma^*$ state. In order to examine the electron donating effect on the ESHT between phenol and ammonia, the cluster of 3-aminophenol (3AP) and ammonia was studied by REMPI and IR-UV double resonance spectroscopy. 3AP has two conformers, *cis* and *trans*, depending on the orientation of the OH group to the amino group, whose electronic origins are well separated. Between the *cis* and *trans* isomers of the bare 3AP, only *trans* isomer was found for $3AP(NH_3)_1$. Complete quenching of the excited state of *cis* isomer, e.g. by conformer-specific ESHT, does not seem to occur. Rather, efficient conformational cooling produces only the more stable *trans* isomer. The 0-0 band of the *trans*-$3AP(NH_3)_1$ at 34409 cm^{-1} is red-shifted by 68 cm^{-1} from that of the *trans*-3AP at 34477 cm^{-1}. The IR depletion spectrum shows that the OH stretching vibration (3296 cm^{-1}) is red-shifted by 362 cm^{-1} from that of the monomer. The large red-shift in OH frequency, combined with MP2 calculation, reveals that the ammonia is bound to the hydroxyl group of 3AP. Since the 0-0 band of 3AP at 34477 cm^{-1} is closer to that of aniline (34048 cm^{-1}) than that of phenol (36360 cm^{-1}), the amino group has larger effect in the electronic transition of the aromatic ring than the hydroxyl group. Thus solvation on the hydroxyl group has a very small effect on the electronic transition of 3AP, leading to a very small red-shift in electronic transition (68 cm^{-1}) compared to phenol-ammonia (650 cm^{-1}).

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발표종류: 심포지엄, 발표일시: 목 15:20, 좌장: 최명룡

Ultraviolet Photodepletion Spectroscopy of Dibenzo-18-Crown-6-Ether Complexes with Alkali and Alkaline Earth Metal Cations

김남준

충북대 화학과

Ultraviolet photodepletion spectra of dibenzo-18-crown-6-ether complexes with alkali and alkaline earth metal cations (M+- and A2+-DB18C6, M=Cs, Rb, K, Na, Li, and A=Ba, Sr, Ca, Mg) were obtained in the gas phase using electrospray ionization quadrupole ion-trap reflectron time-of-flight mass spectrometry. The spectra exhibited a few distinct absorption bands in the wavenumber region of 35450-37800 cm-1. The lowest-energy band was tentatively assigned as the origin of the S0-S1 transition. The red-shifts of the origin bands were observed in the spectra as the size of the metal cation in DB18C6 complex ions increased from Li+ to Cs+ and from Mg2+ to Ba2+. The size effects of the metal cations on the geometric and electronic structures, and the binding properties of the complexes at the S0 and S1 states were elucidated by theoretical calculations using density functional and time-dependent density functional theories. We found a strong correlation between the red-shift in the spectra and the binding energy of the metal cation to DB18C6 at the electronic ground state. This correlation was also observed in the solution-phase absorption spectra between the shift of the lowest absorption band and the stability constant of a metal cation in solution. This study manifests the importance of the gas-phase study revealing the intrinsic properties of molecules and ions to understand the complicated phenomena observed in the condensed phase.

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발표종류: 심포지엄, 발표일시: 목 15:55, 좌장: 류순민

Intramolecular Chemical Reaction Dynamics by Impulsive Excitation of Molecular Vibrations

주태하

포항공과대 화학과

We report the observation of the coherent wave packet motions of the molecules in the excited states created by various processes such as chemical reactions, internal conversion from S_n ($n \geq 2$) to S_1, and Franck Condon transition. The observation of coherent molecular vibrations in the product state gives direct information on the structures of the excited states and the reaction coordinates by examining the modes excited. We use femtosecond time-resolved spontaneous fluorescence (TRF), although typical time resolution of the TRF measurement is limited to around 200 fs, which is not high enough to observe coherent vibrational motions. By the advances made in our laboratory, we can achieve 30 fs time resolution in TRF, which allows direct observation of the vibrational wave packet motions in the excited state. Some examples of such impulsive excitation to the excited state and subsequent observation of the wave packet motion will be presented; direct electronic excitation by the pulsed light, excited state intramolecular proton transfer, and intramolecular charge transfer reactions.

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발표분야: 분자구조 및 화학반응동력학:물리화학자의 관점
발표종류: 심포지엄, 발표일시: 목 16:20, 좌장: 류순민

Quantum Control based on Adiabatic Passage

신석민

서울대 화학부

With the introduction of strong lasers, selectivity and robustness in optical control have been major research interests. Adiabatic passage (AP) process can provide robust and stable control scheme without the needs for considering fluctuations in the experimental parameters. In the control scheme based on Stark-Chirped Rapid Adiabatic Passage (SCRAP), one uses laser-induced Stark-shift as a controllable experimental parameter. We extended SCRAP scheme to selective population transfer in molecular systems, whose dynamics involve dissociation and recombination. The results of these studies illustrate the feasibility of the scheme in complicated systems with practical and reasonable parameters. We also investigated the possibility of using quantum control based on adiabatic passage for constructing a quantum computation scheme.

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발표분야: 분자구조 및 화학반응동력학:물리화학자의 관점
발표종류: 심포지엄, 발표일시: 목 16:45, 좌장: 류순민

Ultrafast X-ray Absorption Spectroscopy of Spin-crossover Dynamics in Solvated Transition Metal Complex

조하나, 김태규

부산대 화학과

We report measurements of the photoinduced Fe^{II} spin crossover reaction dynamics in solution via time-resolved x-ray absorption spectroscopy. EXAFS measurements reveal that the iron-nitrogen bond lengthens by 0.21±0.03 Å in the high-spin transient excited state relative to the low-spin ground state. XANES measurements at the Fe L-edge show directly the influence of the structuralchange on the ligand-field splitting of the Fe^{II} 3*d* orbitals associated with the spin transition. Our experimental approach opens the door to femtosecond x-ray absorption investigations of liquid phase chemistry that have previously been inaccessible.

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발표분야: 나노포토닉스 및 나노분광학
발표종류: 심포지엄, 발표일시: 목 14:00, 좌장: 정영미

Surface-Enhanced Raman Scattering Based Protein Detection

Yukihiro Ozaki, Xiaoxia Han, *Bing Zhao

*Department of Chemistry, Kwansei Gakuin University, Japan *State Key Laboratory of Supramolecular Structure and Materials, Jilin University, China*

Protein studies can give a much better understanding of an organism than genomics, since proteins are main components of the physiological metabolic pathways of cells. It is all-important to design new detection methods for the rapid development of proteomics.Surface-enhanced Raman scattering (SERS) technique has proved to be an effective analytical tool due to its high sensitivity, high selectivity and fluorescence quenching properties. Our objective is to develop simpler and more effective detection methods for proteins with different purpose based on the combination of conventional detection methods and SERS.In most SERS-based studies, SERS-active substrates are usually first prepared (e. g., metal electrodes, or island films), and then analytes are assembled on these substrates for further SERS detections. In our studies, we mainly use a contrary way, which is based on strong interactions between proteins and silver nanoparticles.

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Investigations on Semiconductor-based SERS

Bing Zhao, Libin Yang, Xiangxin Xue

State Key Laboratory of Supramolecular Structure and Materials, Jilin University, China

We has observed SERS signals from molecules adsorbed on pure wide band gap semiconductors like ZnO and TiO2, and proposed the TiO2-to-molecule charge transfer (CT) mechanism. To further improve SERS properties of TiO2 and verify the validity and universality of the observed TiO2-to-molecule CT mechanism, Zn doped TiO2 NPs with various content of Zn were prepared and employed as SERS-active substrates. The results show that SERS performances of TiO2 NPs can be significantly improved by doping with an appropriate amount of Zn. The surface-deposited Ag on TiO2 can inject additional electrons into molecules adsorbed on TiO2 surface through the conduction band of TiO2 NPs, besides the intrinsic TiO2-to-molecule CT contribution. The semiconductor-based SERS is expected to be valuable not only in developing semiconductors as novel SERS substrates but also in exploring adsorption-related problems (the interaction and CT between molecules and semiconductor) on semiconductor surfaces for optimizing the performance of these materials.

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발표분야: 나노포토닉스 및 나노분광학
발표종류: 심포지엄, 발표일시: 목 15:00, 좌장: 정영미

Functionalization and Chemical Properties of Graphene

류순민

경희대 응용화학과

Atom-thick graphene membrane holds substantial potential for applications in future molecular-scale integrated electronics, transparent conducting membranes, nanocomposites, etc. To realize this potential, chemical properties of graphene need to be understood and functionalization toolkits are also required. To meet this need, surface chemistry of graphene has been explored by Raman spectroscopy, AFM and STM scanning probes. In the first part of the talk, two chemical reactions of graphene will be presented. Hydrogenation, the simplest basal plane functionalization, is highly reversible and strongly dependent on the thickness of graphene in the rate. Graphene sheets can be locally hydrogenated with a high spatial resolution. Thermal oxidation also proceeds at a higher rate for single layer than double layer graphene and triple layer graphene behaves like bulk graphite. The second part of the talk will illustrate the influence of underlying silicon dioxide substrates and ambient gases on properties of graphene. Raman spectroscopy shows that freestanding graphene is essentially charge-neutral implying that the “usual” hole-doping in supported graphene is mediated by oxide substrates. An STM study reveals that thermal annealing generates out-of-plane deformation of nanometer-scale wavelength and distortion in sp2 bonding on an atomic scale. Graphene deformed by annealing is found to be chemically active enough to bind molecular oxygen, which leads to a strong hole-doping. A possible form of oxides will be discussed.

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Growth direction determination of a single RuO2 nanowire by polarized Raman spectroscopy

김명화

이화여대 화학 나노과학과

We present the polarization dependence of Raman scattering study of a single crystalline ruthenium dioxide (RuO2) nanowires to explore its use in determining the crystal growth direction as a complementary technique to High Resolution Transmission Microscopy (HRTEM). The results unambiguously indicate that the polarization dependence of the Eg Raman band at 525 cm-1 and the B2g Raman band at 714 cm-1 of a single RuO2 nanowires is highly consistent with its theoretical calculation, which predicts the nanowire growing the (001) crystallographic direction along the c axis of the nanowire. Furthermore, High resolution TEM measurements confirm that RuO2 nanowires are exactly grown along the (001) crystallographic growth direction.

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Stimulated Raman Scattering for Quantitative Analysis

김형민

한국화학연구원 융합바이오기술연구센터

Stimulated Raman Scattering (SRS) is one of the most sensitive Raman techniques which enable to overcome the sensitivity limit of conventional Raman system. Recent advance in state-of-the art laser technology implements the stable SRS method in various field of science. We have been developing broadband stimulated Raman scattering technique which enables rapid monitoring of chemical component. Furthermore chemometrics algorithms (Principal Component Regression, Partial Least Square) are combined with SRS techniques for quantitative analysis.

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발표코드: **금12E1심**
발표분야: RoHS 관련 규제 물질에 대한 분석법 표준화 연구 및 동향
발표종류: 심포지엄, 발표일시: 금 09:00, 좌장: 류재정

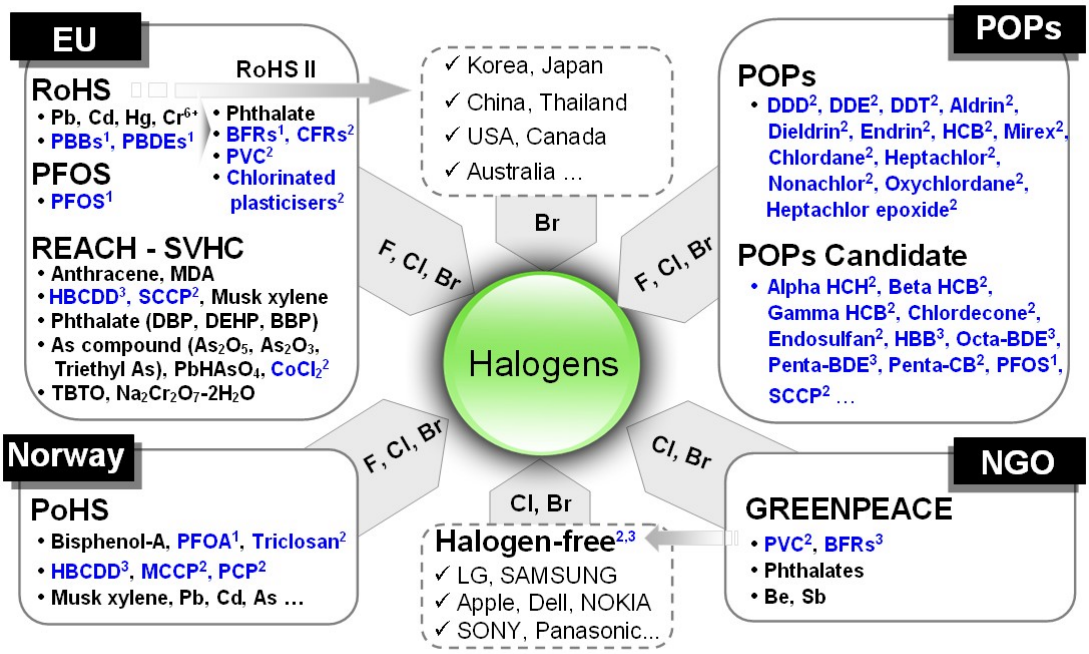
전기전자 제품의 국제환경규제(RoHS, halogen-free) 대응을 위한 시험방법 국제 표준화 사례

정재학

LG Display 구미분석팀

최근 EU 및 각국에서는 잔류성 유기오염물질(POPs), 브롬계 난연제(BFRs), 염소계 난연제(CFRs) 및 과불소화합물(PFOS, PFOA) 등과 같은 각종 유해물질에 대한 규제 차원에서 모니터링을 강화하고 있으며, 대표적인 NGO 인 그린피스의 경우 PVC 및 BFRs 과 같은 물질을 사용하는 전세계 기업체 뿐만 아니라 전세계 주요 전자업체들의 친환경 수준을 정기적으로 평가하여 인터넷상에 공개함으로써 기업체 및 전세계인들에게 친환경 경영에 대한 필요성을 지속적으로 홍보하고 있다. 이러한 상황에서 전기전자제품에 대한 국제 환경규제 대응을 위해 각국의 전문가들은 IEC TC111 을 조직하여 전기전자제품 및 시스템에 대한 환경 표준화를 추진 중이며, 유해물질 함유 여부에 대한 시험방법 표준을 2008 년 12 월에 IEC 62321 규격을 제정하여 전세계의 RoHS 분야에 적용하고 있다. 한국의 경우 현재 RoHS 및 halogen-free 관련 시험방법에서 매우 중요한 halogen 시험방법을 연소 IC 를 활용하여 2009 년 KS 표준을 제정하였으며, 그 표준을 토대로 IEC TC111 WG3 분야에서 한국 최초로 NWIP(신규 표준)를 제안하였고, 그 노력의 결과 IEC 62321 개정본에 포함되어 2012 년까지 최종 표준화가 진행될 예정이다. 이러한 시험방법의 표준화 활동은 자국에 유리한 국제표준을 등록함으로써 국가산업 발전의 유리한 고지를 선점하는 효과를 기대하고 있다. 참고문헌 1.IEC TC111, IEC 62321 Ed.1: Electrotechnical products – Determination of levels of six regulatedsubstances (lead, mercury, cadmium, hexavalent chromium, polybrominated biphenyls,polybrominated diphenyl ethers)2.111/165/NP, Jaehak Jung, Determination of certain substances in electrotechnical products – IEC 62321 Part 3-2: Screening of total bromine by combustion - ion chromatography (C-IC).

Worldwide Environmental Regulations & Restrictions



(Ref.) [1]: fluorine (F), [2]: chlorine (Cl), [3]: bromine (Br)

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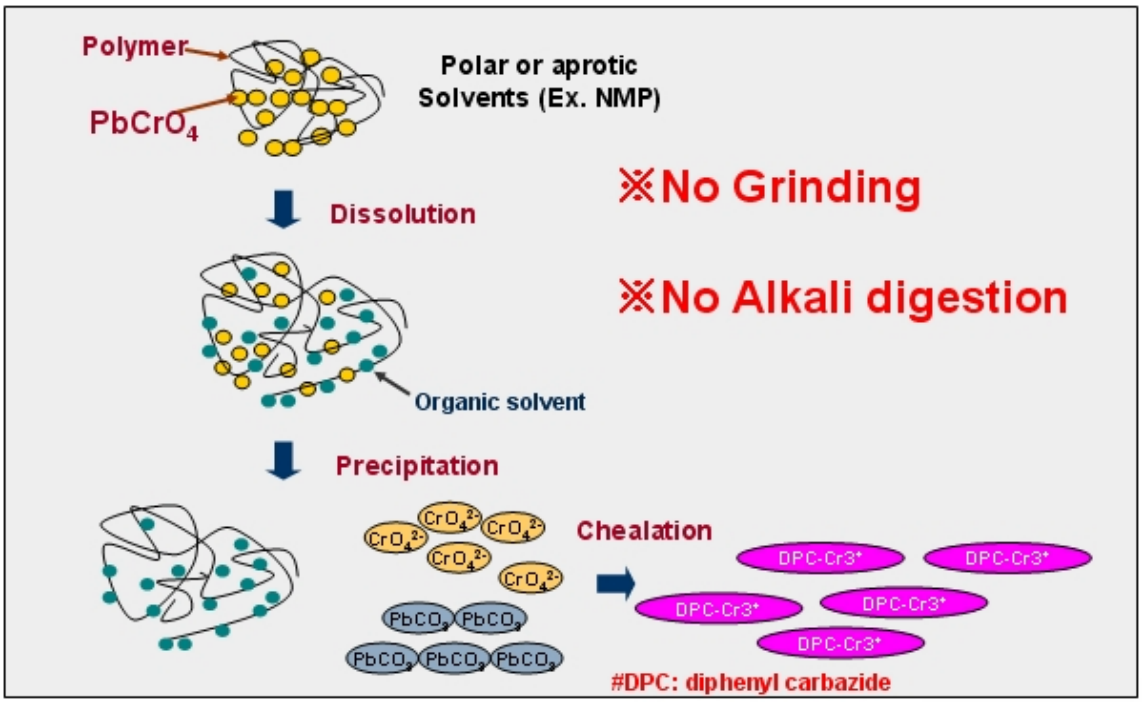
장소: 송도컨벤시아
발표코드: **금12E2심**
발표분야: RoHS 관련 규제 물질에 대한 분석법 표준화 연구 및 동향
발표종류: 심포지엄, 발표일시: 금 09:30, 좌장: 류재정

A novel extraction method using organic solvent dissolution for determination of the hexa-valentchromium in plastic materials

김윤성

제일모직(주) 분석팀

The purpose of this presentation was to improve the efficiency of the alkaline digestion used, according to IEC 62321 standard, to extract Cr(VI) from polymers. The topic of this study is certainly of high interest since increasing industrialization has culminated in a dramatic growth in the volume of plastic materials produced worldwide. A novel method has been developed to fundamentally solve the low recovery% and inefficiency in extracting the Cr(VI) from polymer matrix. Thus, new method allowed the accuracy of the analysis results and speed to maximize. As a result, in recent years there has been great interest for the investigation of possible migration of certain hazardous elements such as Cr(VI) from plastic products



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발표종류: 심포지엄, 발표일시: 금 10:00, 좌장: 류재정

제품환경규제동향 및 SGS의 역할

한재성

SGS 시험사업부

전기 및 전자 산업의 급속한 발전과 더불어 이에 따른 폐기물도 크게 증가하고 있다. 전기 및 전자 장비에 사용된 많은 화학물질이 인체에 유해하거나 유독성이 있으므로 이들 폐기물에서 나오는 새로운 물질 또는 화학물질은 환경에 악영향을 미칠 수 있다. EU 이사회와 유럽 의회는 2003 년 2 월 13 일자로 두 가지 지침(RoHS, WEEE)을 발행했다. 지침의 목적은 전기전자장비 폐기물의 폐기를 통제하고 이러한 제품에 특정 위험 물질의 사용을 제한하는 것이다. EU 로 수입되는 모든 제품은 이 두 가지 지침의 요건을 충족시켜야 한다. 또한 화학물질 및 제품에 대한 환경규제를 더욱 강화하기 위하여최근 REACH 및 EuP 라는 형대의 새로운 형태의 지침도 시행중이다. 따라서 본 논문에서는 EU 시장 요구조건에 초점을 두고 전기전자 산업의 화학분석과 관련된 규정 및 지침을 자세히 설명하고 현재 전반적으로 널리 통용되고 있는 시험방법에 대해 고찰하고자 한다.SGS 를 포함한 global 시험인증기관들은 이러한 제품규제의 충족여부를 검증하는 역할을 하고 있으며 그 규모 또한 점점 커져가고 있다. 각 global 시험기관들의 사업규모 및 주요업무내용에 대해서도 요약 정리하였다. 이러한 글로벌 시험기관들의 적극적인 지원으로 2006 년 7 월부로 EU 에서 적용되고 있는 RoHS 규제에 대한 산업계의 준비는 매우 체계적으로 진행될 수 있었으며, 그 결과 큰 어려움 없이 현재까지 유럽지역 전기전자제품의 수출을 지속할 수 있게 되었다. 그러나 이러한 완벽한 준비는 선도분석기관의 정확한 분석능력에 기인한 바 크며, 앞으로도 이와 같은 분석의 정확성을 유지하는 것이 매우 중요하다.

EU법령	내용	적용시기	적용대상
ELV	폐차처리지침	2003. 7. 1	자동차 및 자동차 부품 생산자
WEEE	폐전기전자제품 지침	2005. 8.13	전기전자제품 생산자
RoHS	전기전자제품 내 유해물질 제한 지침	2006. 7. 1	전기전자제품 생산자
REACH	신물질관리제도	2007. 6. 1	화학물질, 조제품, 완제품 생산자
EuP	에너지사용제품 지침	2009. 11. 1	에너지 사용 또는 변환 제품 중 EU내 연간 20만대 이상 판매제품 생산자

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국제환경규제 대응 분석기술 표준화 동향

이진숙

한국산업기술시험원 재료평가센터

최근 EU 를 선두로 확산되고 있는 제품에 대한 환경유해물질규제는 국내 산업계에 기술무역장벽으로 작용하고 있다. 이러한 동향과 함께 환경유해물질 분석은 환경오염 모니터링을 위한 환경시료 분석에서 전과정 평가를 위한 부품·소재 분석으로, 주요 대상이 전환되고 있다. 아울러 환경규제에 대응하기 위한 기반 기술로서 분석에 대한 일반의 관심이 증폭되고 있으며, 정부 차원에서도 국책 사업으로 분석기술 표준화를 추진하였다. 2002 년부터 최근까지 이와 같은 국책 사업을 통하여 'KS D 2055 EMC 의 납 및 카드뮴 정량방법' 등 관련 국가 표준 60 여 종이 개발되었으며, 이 가운데 일부는 국제 표준으로 제안하여 채택되는 실적을 올렸다. 향후에도 규제물질의 추가 및 규제대상의 확대는 계속될 전망이며, 새로운 기술무역장벽이 국내 기반 기술 발전의 기회요인으로 작용할 수 있도록 국내 분석 전문가들의 네트워크 강화 및 기술력 결집이 요구된다.

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발표종류: 심포지엄, 발표일시: 금 11:10, 좌장: 이용일

Development of Antimony(Sb) Analysis method for Eco-friendly Products

김성일, *신은미

*LS전선 분석연구그룹 *LS전선 중앙연구소*

Ever reinforcing environmental regulations (RoHS, WEEE and ELC, etc.) and increasing demands for eco-friendly products require more strict quality controls on hazardous substances in polymer products including organics and inorganic additives. Antimony trioxide has been used as a flame retardant agent in polymer industry, although its use is more strictly regulated now due to its known adverse health effect. To comply with the customer requirement on Sb contents in plastics, it is essential to develop a validated method to determine antimony contents in polymers with sufficient accuracy and convenience. Screening method for Sb had been developed. The screening method is fast, non-invasive and accurate determination of Sb in polyvinylchloride (PVC) and polyolefin (PO), which are widely used in electric wires. The accuracy was guaranteed using in-house developed reference materials spiked with exactly known amounts of Sb. The consistency and concentration of Sb in WSs were measured by inductively coupled plasma – atomic emission spectrometer(ICP-AES). Moreover, accuracy of HPA preparative method was compared with traditional digestion method & Microwave digestion method.

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발표종류: 심포지엄, 발표일시: 금 11:40, 좌장: 이용일

RoHS 규제 중 난연제 동향 및 분석법 표준화 현황

유석

한국화학시험연구원 정밀화학팀

최근 수출 전자제품의 특정 유해물질 사용규제에 대한 지침(Restriction of Hazardous Substances Directive) 관련하여 환경유해물질에 대한 사용 규제가 점차 강화되고 있는 가운데 현재 6 대물질 (납, 카드뮴, 6 가크롬, 수은, PBBs, PBDEs)이외에 발암•돌연변이•재생독성물질 (CMR, carcinogenity, mutagenicity, toxicity for reproduction), 지속•생물농축•독성물질 (PBT, persistent, bioaccumulative and toxic) 또는 매우 지속성 및 생물농축이 큰 물질 (vPvB, very persistent and very bioaccumulative), 내분비계 장애물질, 기타 브롬계 난연제 등의 후보물질에 대해서도 규제가 추가 될 예정이다. 이에 따라 분석기관의 표준화 시험법 연구도 활발한 추세에 있으며 현재 6 대 규제물질에 대한 시험소의 KOLAS 인증도 확대 시행 중이며 이에 대한 사례를 나타내었다.또한 현재 난연제의 국내•외 시장동향이 브롬계 및 염소계의 환경규제 영향으로 환경대응형 난연제로 인(phosphorus)계, 수화금속화합물등의 난연제로 대체 하는 추세에 있으나 적용 및 성능구현에 어려움이 있어 지속적 개발 및 투자가 필요한 현실이다.

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발표종류: 심포지엄, 발표일시: 금 09:30, 좌장: 배의영

Discovery of novel and potent inhibitors of beta-ketoacyl-acyl carrier protein synthase by NMR spectroscopy and in silico screening

김양미

건국대 생명공학과

The rise of multidrug-resistant of most bacteria requires the development of new antibiotics. bBeta-Ketoacyl acyl carrier protein synthase (KAS) III is a particularly attractive target in the type II fatty acid synthetic pathway, since it is central to the initiation of fatty acid synthesis. In the present study, we used comparative homology modeling and receptor-oriented pharmacophore-based in silico screening to find the candidates of inhibitors for KAS III from S. aureus, E. coli, and E. faecalis. Binding study of selected compounds was performed by Saturation Transfer Difference (STD) NMR spectroscopy, fluorescence experiments and antimicrobial effect was evaluated against various antibiotic-resistant bacteria. From this study, we found several potent inhibitors of ecKAS III and efKAS III which showed an antimicrobial effect against E. coli and E. faecalis and we confirmed the importance of KAS III as targets for antimicrobial agents. Acyl carrier protein (ACP) is a small (~9 kDa) acidic protein whose function is essential for numerous biosynthetic pathways that depend upon acyl group transfer. Here, we investigated dynamic properties of ACP through observation of spin relaxation parameters. Backbone dynamics of ACP shows that extensive mobility in α1α2 loop and the N-terminal residues exhibit a conformational exchange process. HSQC spectra of holo-ACP showed two sets of resonances, suggesting that two conformers are in dynamic equilibrium. However, acyl-ACP has only one set of resonances. NMR data of acyl-ACP revealed that changes in the length of the covalently attached fatty acid affect the local conformation and the dynamics of ACP. Flexibility of ACP shown in this study is essential for its ability to interact with functionally different enzyme partners including KAS III in fatty acid synthetic pathway of bacteria.

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발표종류: 심포지엄, 발표일시: 금 09:55, 좌장: 배의영

Role of ubiquitin in neuroprotection

유권열

서울시립대 생명과학과

Pathogenesis of neurodegenerative diseases, such as Alzheimer's and Huntington's diseases, is linked to the accumulation of non-native protein aggregates or inclusion bodies, which are pathological hallmarks of these disorders. In addition, abnormal accumulations of ubiquitin (Ub) within neuronal inclusion bodies have been diagnostic features of nearly all neurodegenerative diseases. Although it is clear that these diseases are associated with the accumulation of ubiquitinated aggregates, it has not been extensively studied how it leads to neuronal loss or dysfunction. Our hypothesis is that the formation of ubiquitinated aggregates disrupts Ub pool dynamics by shifting the Ub pool equilibrium towards Ub conjugates and reducing the availability of free Ub, which is associated with diverse neurological disorders. In our previous study, we have demonstrated that modest depletion of cellular Ub is sufficient to cause neuronal dysfunction and neurodegeneration. Therefore, the goal of this project is to identify the role of Ub in regulating neuronal function and survival. To this end, we determined the spatial profiles of polyubiquitin gene (*Ubb* and *Ubc*) expression patterns and their contribution to total Ub levels in mouse brain under normal and stressed conditions. Next, we will determine whether free Ub levels are reduced and Ub pool dynamics are disrupted in the affected brain regions where inclusion bodies are formed using selected aging-related mouse models of neurodegeneration, and we will rescue neuropathological lesions by providing extra free Ub via lentiviral-mediated delivery. This will directly prove the neuroprotective role of Ub and eventually identify underlying molecular mechanisms why Ub deficiency in neurons causes neuronal loss or dysfunction leading to various neurological disorders. This work is supported by a grant from the Korea Health Industry Development Institute (A084520).

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Protein engineering of Coprinus cinereus peroxidase for the application to polymerization of phenolics

김용환

광운대 화학공학과

The peroxidase has been commonly used in many biotechnology fields, from fine chemical synthesis to environmental clean-up. The peroxidase catalyzes the oxidation of phenolic compounds. Two equivalents of phenol are converted into a highly reactive radical species by each consuming one equivalent of hydrogen peroxide. The CiP was significantly inactivated during the oxidation of phenolic compounds. Conversely, the CiP nearly maintained its initial activity for the oxidation of syringic acid, vanilic acid and ferulic acid. The thermodynamic parameter (ΔΔG_f298K) and turnover capacity (ΔS/ΔE) were adapted to explain the CiP inactivation due to covalent bonding between the enzyme and phenolic compounds. In the cases of syringic acid, vanilic acid and ferulic acid, which maintained high residual CiP activities after reaction, the ΔΔG_f298K^0 were more negative and the turnover capacities were higher than the other values. This means that these compounds prefer to form a dimer rather than an enzyme-phenolics complex. Among the inactivation factors, the formation of covalent bonding between the enzyme and phenolic radicals was concluded to be the main mechanism for the inactivation of CiP. The sequence of fragment from inactivated CiP (m/z 838.880) was KGTTQPGPSLGFAEELSPFPGEFRM (residues 219-241, underlined residue F229) and was covalently modified with molecular phenol, whereas a fragment of native CiP (m/z 1211.621) was not. Various mutants of the F229 residue of CiP were constructed to investigate the possibility to block the inactivation caused by radical coupling of phenols with the Phe residue through site directed mutation and expressed in Pichia pastoris by using pPicZA as expression vector. The F229A mutant showed a higher turnover capacity (14 fold higher than that of wild-type) and both the F229I and F229L mutants showed an increase in the turnover capacity of 5 fold. Herein, we proposed that the major inactivation mechanism for CiP is the attack of the F229 residue of CiP by the radical. This attack can form a covalent bond between the phenolic radical and the enzyme. The modified F229 with the phenol polymer at the entrance of active

pocket then blocks the active center, which may be called “molecular clothing or shielding”. This work provides a more detailed understanding of the suicide inactivation of peroxidase and suggests the strategy for the development of stable peroxidase against the oxidation of enzyme itself. The radical-resistant robust peroxidase can be efficiently used in diverse fields, from the analytical diagnostic field as a key component of biosensors and immunoassays to the industrial processes as a biocatalyst in the synthesis of fine chemicals including phenolic polymers.

대 한 화 학 회
THE KOREAN CHEMICAL SOCIETY

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발표종류: 심포지엄, 발표일시: 금 11:00, 좌장: 유권열

An Emerging Protein Phosphatase - The Kinetic and Structural Study

김영준

건국대 응용생화학과

Phosphorylation and dephosphorylation of the C-terminal domain (CTD) of RNA polymerase II (Pol II) represent a critical regulatory checkpoint for transcription. Transcription initiation requires Fcp1/Scp1-mediated dephosphorylation of phospho-CTD. Fcp1 and Scp1 belong to a family of Mg2+ -dependent phosphoserine (P.Ser)/phosphothreonine (P.Thr)-specific phosphatases. We present the X-ray crystal structures of a dominant-negative form of human Scp1 (D96N mutant) bound to mono- and diphosphorylated peptides encompassing the CTD heptad repeat (Y1S2P3T4S5P6S7). Moreover, kinetic and thermodynamic analyses of Scp1-phospho-CTD peptide complexes support the structures determined. This combined structure-function analysis discloses the residues in Scp1 involved in CTD binding and its preferential dephosphorylation of P.Ser5 of the CTD heptad repeat. Moreover, these results provide a template for the design of specific inhibitors of Scp1 for the study of neuronal stem cell development. Scp1 is a member of haloacid dehalogenase (HAD) superfamily, whose catalysis depends on a Mg2+ ion and a DXDX(T/V) motif, both of which are signature features of HAD super family members. The first Asp of the motif is identified to be the nucleophile that is subjected for phosphorylation leading to a phosphoryl-aspartate intermediate. This high-energy mixed anhydride intermediate is subsequently hydrolyzed to regenerate the enzyme. The proposed mechanism for Scp1 is widely accepted, however, the phosphoryl intermediate has never been captured directly in Scp1 or its closed family members. In the present study, we successfully captured the phosphoryl-aspartate intermediate in the crystal structure of Scp1 D206A mutant soaked with para-nitro phenyl phosphate (pNPP), providing confirmative evidence for the proposed two-step mechanism. Furthermore, steady-state kinetic analysis of a variety of Scp1 mutants revealed the Mg2+-coordinating function of Asp206, a conserved residue in HAD superfamily whose role was not noticed before. Our results strongly suggest that Asp206 and its equivalent residues in other HAD family members play a structural and mechanistic role. This study laid the foundation for future studies on the mechanism of Scp1 and other HAD family members.

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발표종류: 심포지엄, 발표일시: 금 11:25, 좌장: 유권열

Engineering Protein Thermal Stability: Biochemistry, Biophysics, Computation and Bioinformatics

배의영

서울대 농생명공학부

Engineering proteins for higher thermal stability remains an important but difficult challenge. Clues to designing more stable proteins can be obtained by comparing and contrasting natural proteins from thermophiles, mesophiles and psychrophiles. Three such adenylate kinases were studied to reveal sequential and structural differences responsible for their disparate thermal stabilities. To obtain detailed information about their structures and dynamics, experimental and computational techniques were used. Their crystal structures were solved by X-ray crystallography and their dynamics were studied using molecular dynamics simulations. Based on comparative analysis of the structures and simulations, specific molecular mechanisms for their different thermal stabilities were proposed and tested by in vitro and in silico analysis of mutant enzymes. To further distinguish the roles of specific structural domains in stability and catalysis of adenylate kinase, chimeric enzymes were developed from the thermophilic and mesophilic adenylate kinases. Using a new method with synthetic genes, a series of chimeras were efficiently generated with specific regions exchanged. Analysis of the chimeras revealed that stability and activity were controlled by different domains in adenylate kinase. A bioinformatic method has also been developed to redesign proteins to be more stable through optimization of local structural entropy. The redesigned proteins display significant increases in their thermal stabilities while retaining catalytic activity, and demonstrate a broadly applicable method.

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Hsp90 chaperone machinery in cancer and immunity

한지숙

서울대 화학생물공학부

Hsp90 is one of the most abundant molecular chaperones in eukaryotic cells, playing an important role in folding, stabilization, activation, and assembly of metastable 'client' proteins which include many oncogenic proteins. Inhibition of Hsp90 leads to simultaneous degradation of the oncogenic client proteins, placing Hsp90 as a promising new target for anti-cancer drug development. To identify novel classes of Hsp90 inhibitors, we utilized structure-based virtual screening of a chemical database with docking simulations in the N-terminal ATP-binding site of Hsp90, in vitro ATPase assay of yeast Hsp90, and cell-based Her2 degradation assay in a consecutive manner. As a result, we identified Hsp90 inhibitors with noble scaffolds which exert anti-proliferative effect on MCF-7 breast cancer cells. We also developed a novel tool to detect interaction between Hsp90 and Hsp90 inhibitors based on carboxylated polypyrrole nanotube (CPNT) field-effect transistor (FET) platform. The resulting platform allowed sensitive and specific detection of Hsp90 inhibitor binding to Hsp90 in real-time. Accumulating evidence suggests that Hsp90 is also involved in innate immune response by regulating various signaling molecules including NLRs (Nod-like receptors). We will discuss the biochemical analyses of a novel Hsp90 chaperone complex containing two co-chaperones, Chp-1 and of protein phosphatase 5 (PP5), which is a potential regulator of NLRs.

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발표분야: 바이오 활용 나노기술과 의약기술
발표종류: 심포지엄, 발표일시: 목 14:00, 좌장: 하상수

Large-scale Synthesis of Uniform-sized Nanocrystals and their Designed Assembly for Multifunctional Biomedical Applications

현택환

서울대 화학생물공학부

We developed a new generalized synthetic procedure, called as “heat-up process,” to produce uniform-sized nanocrystals of many transition metals and oxides without a size selection process (see review article: Angew. Chem. Int. Ed. 2007, 46, 4630). Very recently we were able to synthesize uniform oxide nanocrystals as much as 1 kilogram-scale from the thermolysis of metal-oleate complexes. Clever combination of different nanoscale materials will lead to the development of multifunctional nano-biomedical platforms for simultaneous targeted delivery, fast diagnosis, and efficient therapy. In this presentation, I would like to present some of our group’s recent results on the designed fabrication of multifunctional nanostructured materials based on uniform-sized nanoparticles and their bio-medical applications. We developed a new T1 MRI contrast agent using biocompatible manganese oxide (MnO) nanoparticles, exhibiting detailed anatomic structures of mouse brain. We reported on the fabrication of monodisperse nanoparticles embedded in uniform pore-sized mesoporous silica spheres and PLGA polymers for simultaneous MRI, fluorescence imaging, and drug delivery. We used ferromagnetic iron oxide nanocrystals for T2 MRI contrast agent for tracking transplanted pancreatic islet cells. We synthesized hollow magnetite nanocapsules and used them for both the MRI contrast agent and magnetic guided drug delivery vehicle.

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발표종류: 심포지엄, 발표일시: 목 14:30, 좌장: 하상수

RNA Grooves Can Accommodate Disulfide-Bridged Bundles of alpha-Helical Peptides

유재훈

서울대 화학교육과

A strategy for chemical stapling increases structural as well as chemical stability of helical peptides. Using an amphiphilic peptide with Leu/Lys, two Leu residues were replaced by Cys. Helical bundle peptides were generated by oxidative disulfide bond formation. One of these has a Kd as low as 21 picomolar against hairpin targets. This observation demonstrates that the groove in small hairpin RNA has sufficient room to contain a helical bundle peptide.

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발표분야: 바이오 활용 나노기술과 의약기술
발표종류: 심포지엄, 발표일시: 목 15:00, 좌장: 하상수

Theragnostic Chiotsan-based Nanoparicles for Cancer Imaging and Therapy

김광명

KIST

Herein, we report that a new nano-sized carrier of tumor-homing chitosan-based nanoparticles (CNP) that can be used not only as nano-sized carriers of an anticancer drug (Paclitaxel; Dodetaxel, doxorubisin, photosensitizer, so on), but also nano-sized imaging probes for in real-time tracking CNPs in live animals. With the help of optical imaging technology, the in real-time and non-invasive destination of CNPs in live animal was monitored to elucidate mechanisms responsible for the targeting efficacy, in vivo biodistribution and optimal treatement conditions of CNPs in tumor-bearing mice. The biocompatible and biodegradable CNPs, that contains encapsulated anticancer drugs and near-infrared (NIR) fluorescence (Cy5.5) accumulated selectively and efficiently in tumor and they enhanced the efficacy of the drug against tumor and also reduced its toxicity. This new approach for nano-sized carriers with anticancer drugs and imaging probes simultaneously may provide a new strategy for rational design of cancer diagnostics and therapy (cancer theragnosis), allowing early detection and then followed by effective targeted therapeutics.

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Self-Assembling Bioactive Peptide Nanomaterials

임용범

연세대 신소재공학과

Research on nanometer-sized structures has become one of the fastest growing fields of science & engineering. From the standpoint of biological system, submicron-sized nano-objects are generally much smaller than most cells, but are similar in size to many subcellular components, cellular organelles, and microorganisms such as viruses. Most eukaryotic cells have the typical size of a few tens of microns in diameter. Therefore, the nano-sized biological objects can be regarded as ‘biological nanostructures’ as compared to "synthetic nanostructures" or "artificial nanostructures". Supramolecular or self-assembling synthetic nanostructures covered with bioactive functional molecules have been actively explored as promising nanobiomaterials. Recent advances in nano-sized science, combined with appropriate bioactive functionalization, have led to the successful utilization of supramolecular artificial nanostructures in diverse biomaterials applications. Here, our recent effort to develop self-assembling bioactive nanostructures, with special emphasis on peptide nanostructures, will be presented.

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Dexamethasone conjugated polyethylenimine as a carrier of plasmid encoding heme oxygenase-1 for stroke gene therapy

이민형

한양대 응용화공생명공학부

Dexamethasone is one of the anti-inflammatory glucocorticoid steroids. Previously, we synthesized dexamethasone conjugated polyethylenimine (PEI-Dexa) as a gene carrier with anti-inflammatory effect. In this study, HO-1 gene was delivered to focal ischemic brain of stroke animal model using PEI-Dexa as a gene carrier. Heme oxygenase-1 (HO-1) is an anti-apoptotic protein, which can protect cell from apoptosis under hypoxia. In divided groups of rats (n=9), pEmpty/PEI, pEmpty/PEI-Dexa and pSV-HO-1/PEI-Dexa complexes were injected directly into the cortex 1 hr prior to middle cerebral artery occlusion (MCAO) except control group. MCAO was performed for 60 min in male Sprague Dawley (SD) rats (280-320 g). Also, cortical blood flow was continuously monitored by Laser Doppler Flowmetry. At 24 hrs after MCAO, infarct size was evaluated by 2% 2,3,5-triphenyltetrazolium hydrochloride (TTC) staining. The level of cytokines such as TNF-alpha, IL-1beta were measured by ELISA in the infarcted area. ELISA for the HO-1 protein was also performed to evaluate the gene expression level. The results showed that the injection of pEmpty/PEI-Dexa complex reduced infarct size significantly, compared with the control and pEmpty/PEI injection groups. This suggests that dexamethsone segment of PEI-Dexa protects the brain cells under ischemia-reperfusion condition. Also, HO-1 expression was induced in the pSV-HO-1/PEI-Dexa injection group. The infarct size of the pSV-HO-1/PEI-Dexa injection group was further reduced compared with the pEmpty/PEI-Dexa injection group, suggesting that HO-1 has synergistic effect with PEI-Dexa in reducing inflammatory response in ischemic brain. Therefore, pSV-HO-1/PEI-Dexa complex is a potential candidate for therapeutic gene delivery to ischemic brain.

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발표종류: 심포지엄, 발표일시: 목 16:30, 좌장: 하상수

Polyvalent Nanoparticle-Oligonucleotide Conjugates: Synthesis, Properties, and Therapeutic Applications

이재승

고려대 신소재공학부

Polyvalent nanoparticle-oligonucleotide conjugates exhibit a variety of unique features such as programmable assembly and disassembly, sharp melting transitions, intense optical properties, high stability, enhanced binding properties, and easy fabrication of the surface nature by chemical and physical modification. The unique properties of nanoparticle-oligonucleotide conjugates enable one to build up a number of various applications. For example, nanoparticle-RNA conjugates demonstrate great promise of therapeutic applications in the context of RNA interference when combined with polymeric materials. In this presentation, representative examples of various aspects of nanoparticle-oligonucleotide conjugates will be discussed.

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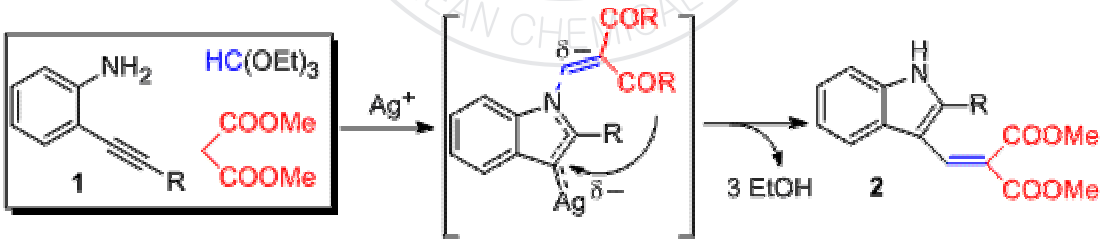
발표분야: 유기화학의 최근 동향: 기초연구개발을 중심으로
발표종류: 분과기념강연, 발표일시: 목 13:30, 좌장: 김종승

Ag-catalyzed Three-Component Green Reaction to Indoles

오창호

한양대 화학과

Indole is a core skeleton in many naturally-occurring alkaloids and some derivatives were licensed for the treatment of inflammation and pain caused by osteoarthritis and rheumatoid arthritis. During developing an atom-economic green reaction, we could find a highly valuable silver-catalyzed three-component reaction of *N*-(2-alkynyl)aniline, triethylorthoformate, and malonate. Mechanistically, this process would involve a new type of 1,3-alkenyl group shift to the silver carbine. In this presentation, I wish to report this novel route concerning 1,3-alkenyl shift leading to 2,3-substituted indoles (2) from the synthetic and mechanistic points of view.



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발표종류: 심포지엄, 발표일시: 목 14:10, 좌장: 하현준

Engineering enzymes to catalyze an unnatural reaction: perhydrolysis

Romas Kazlauskas

University of Minnesota, Department of Biochemistry, Molecular Biology & Biophysics and Seoul National University, School of Chemical and Biological Engineering

Some enzymes, besides catalyzing their normal reaction, also catalyze other reactions. This ability is called catalytic promiscuity. Protein engineering can enhance this promiscuous catalytic activity to create a synthetically useful enzyme. Esterases such as esterase from *Pseudomonas fluorescens*, normally catalyze hydrolysis, but they can also catalyze perhydrolysis to generate a peroxycarboxylic acid. Replacing a leucine in the active site of this esterase with proline enhances perhydrolysis 28-fold and decreases ester hydrolysis 94-fold. The molecular basis of this switch from an esterase to a perhydrolase has been identified as a key hydrogen bond that orients hydrogen peroxide. Other mutations in the active site of this esterase can also increase perhydrolysis, but these have a different, but not clearly understood, mechanism. Perhydrolases can be used make peracetic acid, which can break down lignin in lignocellulosic materials like wood. This pretreatment enhances the release of glucose from the cellulose component of wood and may be useful to produce biofuels.

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발표종류: 심포지엄, 발표일시: 목 14:50, 좌장: 하현준

Palladium-Catalyzed Cross-Coupling Reactions Using Organoindium Reagents

이필호

강원대 화학과

Pd-catalyzed cross-coupling reaction of electrophiles with organometallic reagents is one of the most straightforward methods for C-C bond formation. Among these, reactions using organoindium reagents have came out as a favorite due to its reactivity, selectivity, ease of preparation and handling, operational simplicity, and low toxicity. On the basis of these properties of organoindium reagents, we reported the efficient Pd-catalyzed 1,3-butadien-2-yl cross-coupling reactions using an organoindium reagents generated in situ from the reaction of indium with allenylmethyl bromide, producing a variety of 2-aryl or vinyl substituted 1,3-butadiene derivatives. Moreover, the cross-coupling reactions and subsequent [4+2] cycloaddition provided the rapid synthesis of six-membered carbocycles in a one-pot process. Tandem Diels-Alder/cross-coupling reactions with organoindium reagents generated in situ from 1-bromo-2,3-butadiene and indium were developed in a one-pot process. [4+2] Cycloaddition reactions using organoindium reagents and subsequent Pd-catalyzed cross-coupling reactions provided the rapid synthesis of six-membered carbocycles starting from 1-bromo-2,3-butadiene. In addition, we reported the efficient Pd-catalyzed allenyl cross-coupling reactions using organoindium reagents generated in situ from ethoxycarbonyl propargyl halide.

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The Methodology for the Chemical Synthesis via Catalytic Reactions

김성수

인하대 화학과

Multicomponent synthesis of homoallylic amines and O-acetyl cynohydrines has been reported at rt. Bismuth (III) nitrate pentahydrate ($Bi(NO_3)_3{\cdot}5H_2O$) catalyzes efficiently the three component condensation of aldehydes, amines and allyltributylstannane for the synthesis of homoallylic amines.[1] $B(C_6F_5)_3$ is used as efficient catalyst for the reaction between aldehydes or ketones with TMSCN and acetic anhydride (Ac_2O) to give good to excellent yield of the O-acetyl cynohydrines without solvent at rt.[2] Similarly $B(C_6F_5)_3$ is also applicable for the synthesis of α-aryl nitriles from the corresponding α-aryl alcohols and $(CH_3)_3SiCN$ as cyanide source at rt.[3] Nafion SAC-13[4] and $Bi(OTf)_3$[5] are found to be simple and efficient catalyst for the silylation of alcohols and phenols with HMDS at rt under solvent-free condition. Uncatalyzed method for the silylation of alcohols and phenols with HMDS in CH_3NO_2 is developed at rt.[6] Mild and efficient $InBr_3$-catalyzed Friedel-Crafts alkylation of heteroaromatic or electron-rich aromatic compounds with α-amido sulfones at rt in CH_2Cl_2 has been developed. α-Amido sulfones are employed for the synthesis of the unsymmetrical and bi-symmetrical tri-aryl methanes.[7] Ferric chloride hexahydrate is used as a catalyst for the arylations of α-amido sulfones with electron-rich arenes through Friedel-crafts alkylations.[8] A variety of α-amido p-tolyl sulfones is prepared from aromatic as well as aliphatic aldehydes for the synthesis of α-amino nitriles.[9] A mild and efficient $Fe(ClO_4)_2{\cdot}xH_2O$-catalyzed C-C bond coupling reactions of 1,3-dicarbonyl compounds, electron-rich arenes and heteroarenes, and 4-hydroxycoumarin with secondary alcohols have been described.[10]

Refereneces : **1.**Ponnaboina Thirupathi and Sung Soo Kim, ***Tetrahedron*** **2009**, 65, 5168. **2.**Santosh T. Kadam and Sung Soo Kim, ***Tetrahedron*** **2009**, 65, 6330. **3.**Gurusamy Rajagopal and Sung Soo Kim, ***Tetrahedron*** **2009**, 65, 4351. **4.**Gurusamy Rajagopal, Hanbin Lee and Sung Soo Kim, ***Tetrahedron*** **2009**, 65, 4735. **5.**Santosh T. Kadam and Sung Soo Kim, ***J. Organomet. Chem.*** **2009**, 694, 2562. **6.**Santosh T. Kadam and Sung Soo Kim, ***Green Chemistry*** **2010**, 12, 94. **7.**Ponnaboina Thirupathi and Sung Soo Kim,

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Intelligent chemosensors

윤주영

이화여대 화학과

Fluorescent chemosensors for anions appear particularly attractive due to its simplicity and high detection limit. Imidazolium group can make a strong ionic hydrogen bond with anions . A new water-soluble and fluorescent imidazolium receptor was synthesized as a first ratiometric sensor for ATP, which effectively and selectively recognizes the biologically important ATP over other structurally similar nucleoside triphosphates in aqueous solution of physiological pH 7.4. We recently reported a novel amide-containing receptor for Zn(II), combined with a naphthalimide fluorophore, termed ZTRS. The fluorescence, absorption detection, NMR and IR studies indicated that ZTRS bound Zn(II) in an imidic acid tautomeric form of the amide/di-2-picolylamine 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 Zn(II) over most competitive HTM ions. Finally, a new polymer based on PDA and imidazolium showed a selective color response to anionic surfactants.3 Furthermore, by this system, it is easy to distinguish two different anionic surfactants sodium dodecyl sulfate (SDS) and sodium dodecylbenzenesulfonic acid (SDBS).

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Tracking Quantitative Substrate Preferences of Ru and Mo Catalysts for Metathesis Reactions Using Fluorescence Quenching

손정훈

한국파스퇴르연구소 ACS Team

Great advances have been made in terms of synthetic applications of the metathesis reactions but there are still ambiguities in the mechanistic understanding, with the most salient unresolved fundamental issue being the substrate preference of a catalyst. Although association of a catalyst with its substrate can dictate the identity of the initial adduct or intermediate that directs the reaction pathway and the ultimate key propagating species, even substrate-association preference of this famous class of catalysts has not been well characterized. In particular, the reaction initiation in ring-closing enyne metathesis has been a long lasting controversy. Due to the dearth of knowledge on the substrate preference, it could not be established how much the molecular identity of metathesis catalysts influences their substrate preferences and thus whether each catalyst directs different reaction pathways in the presence of multiple substrates. We have quantified the catalyst-substrate interactions in metathesis reactions using FRET-based method, which afforded quantitative association preferences of the representative metathesis Ru and Mo catalysts to their substrates, alkene, alkyne and allene. The determined substrate preferences are proved to be dependent on the molecular identity of the catalyst and the results provide new insight into the metathesis reactions along with answering the reaction initiation in enyne metathesis and previously unexplained metathesis patterns.

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발표종류: 심포지엄, 발표일시: 금 13:30, 좌장: 이원구

Selective MAP Kinase Cascade Blockers

심태보

KIST 생명보건본부

The mitogen-activated protein kinase (MAPK) pathway composed of Ras/Raf/MEK/ERK governs fundamental cellular signaling network such as proliferation, differentiation and survival. The MAPK signaling pathway has thus received an enormous amount of attention as one of the most promising molecular targets of cancer therapeutics. In the first part of this talk, pharmacological profile of novel Raf-V600E kinase inhibitor identified by my group will be briefly presented in the view of drug discovery. L-783277, naturally occurring 14-membered resorcylic acid lactone exhibited high potency against MEK and ERK with reasonable kinase selectivity. The enantioselective total synthesis of natural product, L-783277 will be discussed along with biological profiles of L-783277 and its derivatives in the second part of this presentation.

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Synthesis of the major metabolites of an ER alpha selective, dihydrobenzoxathiin antagonist for osteoporosis

seongkon kim

종근당 의약화학 및 공정개발실

In conjuction with a medicinal chemistry program targeting selective estrogen receptor modulatiors (SERMs), dihydrobenzoxathiin was discovered to be a potent SERAM that exhibited subnanomolar binding to Er alpha and 40-fold selectivity. Further evaluation of the compound revealed its promise for the prevention of estrogen-deficiency osteopenia in postmenopausal women, without uterotropism, and thereby the compound qualified as a developmental candidate. In preclinical studies in the rhesus monkey, the major metabolites of the parent compound included two O-glucuronides and the bridge compound, which together accounted for approximately 70% of the metabolism. The intriguing biotransformation was confirmed by a 19 step total synthesis starting from resorcinol, the key of which was the construction of the oxygen bridge utilizing a phenolic oxidation and trapping sequence.

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제약산업에서 공정개발의 동향 및 실제

김남두

한미약품 연구센터

유기화학 전공자가 제약산업에서 하는 일은 유기합성을 통해 크게 신규 물질을 만드는 일, 즉 신약개발과 API(an Active Pharmaceutical Ingredient)를 산업화시킬 수 있게 경제적인 합성공정을 개발하는 일, 공정개발로 두 가지로 나눌 수 있다. 신약개발은 유기화학 전공자들의 로망이 되었지만 공정개발은 잘 알려져 있지 않은 면이 있다. 그러나 오늘날 약물의 구조가 복잡해지고, 생산단가에 대한 압박은 점점 거세지고 있다. 또한 약물에 대한 허가규정은 매우 까다로워지고, 환경문제 또한 중요한 해결과제가 되어가고 있는 오늘의 상황에서 공정개발의 중요성은 제약산업에서 점점 더 커지고 있다. 본 세미나에서는 최근의 공정개발의 동향을 2006 년 당뇨병의 치료제로 허가된 시타글립틴의 개발과정을 통해서 보여드리고자 하며, 상대적을 신약이 적은 국내의 상황에서 어떤 노력을 하고 있는지를 항암제인 도세탁셀의 개발 예를 들어 보여드리고자 한다.

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OLED용 유기 발광 재료의 개발 현황

김봉옥

다우어드배스드디스플레이머티리얼 연구소

OLED(Organic Light Emitting Diode)는 LCD 대비 우수한 화질 특성과 간단한 소자 구조 등의 장점을 가진 가장 촉망받는 차세대 디스플레이이다. AMOLED 는 각종 휴대기기를 시작으로 이제 막 상용화를 시작하였으며, 향후 몇 년간 눈부신 성장세를 보일 것으로 예측되고 있다. OLED 는 1987 년 처음 개념이 발표된 이래 그 산업가능성에 주목하여 매우 빠른 속도로 상용화가 추진된 분야이며, 최초로 상용화된 유기물 기반의 전자 기기이기도 하다. OLED 산업의 성장은 향후 전개될 유기물 기반의 전자 산업이라는 새로운 세대의 시작을 보여주는 것이라 하겠다. OLED 는 전극 사이에 다층 유기박막으로 이루어진 매우 간단한 구조이며, 전기장을 걸면 양극으로부터는 정공이, 음극으로부터는 전자가 유입되어 소자의 중심부에서 정공과 전자가 만나 exciton 을 이루고, 정공과 전자가 재결합될 때 여분의 에너지를 빛으로 방출하는 원리를 이용하는 것이다. 사용되는 유기 재료의 전기 광학적 특성, 다층 박막의 인접한 재료간의 계면 특성이 OLED 의 발광 효율, 소자 수명, 발광색상 등 중요한 특성을 결정한다. 그러므로 OLED 산업에서 우수한 성능을 갖는 유기 재료의 개발은 가장 중요한 기술 요소라 할 것이다. 본 발표에서는 OLED 에 사용되는 각종 유기 재료의 개발 방향과 Dow 의 OLED 재료 연구 개발 활동을 소개하고자 한다.

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Organic Materials in Hybrid Nanostructures for optimized functionality

정현민

한국화학연구원 화학소재연구단 정보전자폴리머연구센터

Fabrication of organic-inorganic hybrid materials with controlled nanostructures has been intensively developed to have various structures and properties allowing them to function as high and low dielectric materials in use of electronic devices. In this work, an importance of controlling organic layers in hybrid materials is described, in which the organic-inorganic interfaces significantly affect the dielectric properties. The organic functional groups are introduced in polymeric materials to form the covalent bonding on inorganic nanoparticles. Also, the transformations of functional groups in fabrication process provide a variable layer structure in core-shell hybrid particles. The resulting core-shell particles with robust and stable organic shielding layers show excellent dielectric properties with low current leakage which is hardly found in conventional organic-inorganic composite materials.

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Self-assembling Organic Materials based on Dendritic Building Blocks

조병기

단국대 화학과

본 연구실에서 서로 다른 빌딩블록들의 (덴드론, 막대, 디스크 등등) 융합을 통해 다양한 혼성구조를 갖는 유기화합물들을 합성하여, 나노 구조제어를 통한 기능성 물질 제조에 대해 연구하고 있다. 최근에는, 빌딩블록들의 혼성화를 보다 용이하게 하기 위하여, 많은 연구자들이 사용하고 있는 클릭반응을 도입하여 다양한 분자구조체들을 설계할 수 있었다. 특히, 단순히 블록간의 연결에 관심이 있었던 기존의 연구와는 다르게, 본 연구실에서는 클릭 반응을 통해 생성되는 triazole 그룹의 방향족 특성 및 기능성에 초점을 맞추어 연구를 진행하였다. 본 발표에서는 덴드리틱 빌딩 블록을 함유하는 혼성 유기화합물들의 자기조립 초분자구조형성에 대해 논의하고, 더불어 클릭화학을 이용한 새로운 형태의 자기조립 분자체에 대해서도 소개하고자 한다.

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Current Therapies and Emerging Approaches to the Treatment of Type 2 Diabetes

김두섭

카이노스메드

Type 2 diabetes is a growing public health problem, affecting approximately 150 million people worldwide and the prevalence of type 2 diabetes is expected to reach 366 millions by 2030. Three major therapies to treat type 2 diabetes include stimulating insulin secretion with sulfonylurea, lowering hepatic glucose overproduction with biguanides, and improving insulin resistance with glitazones. Although these therapies have proven therapeutically beneficial, these often show undesirable side effects such as hypoglycemia, drug-drug interactions, lactic acidosis, edema, and weight gain. 30-40% of diabetic patients are not adequately treated with these agents and inadequate long term durability and efficacy are major problems with these therapies. Thus, there are clearly unmet medical needs. Recently, inhibition of dipeptidyl peptidase IV (DPP-4), a serine protease, has emerged as a new approach to the treatment of type 2 diabetes. DPP-4 inhibitors function as indirect stimulators of glucose-dependent insulin biosynthesis and secretion and these effects are believed to be mediated primarily by enhancing the action of an incretin hormone, glucagon-like peptide 1 (GLP-1). In this presentation a new therapy based on the inhibition of DPP-4 as well as emerging new approaches to the treatment of type 2 diabetes targets will be discussed.

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Discovery of a novel non-brain penetrating CB1 receptor antagonist as an anti-diabetic agent

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Type-2 diabetes is related to abdominal obesity and is associated with other cardiometabolic risk factors. Several animal and human observations suggest that the endocannabinoid system is over-active in the presence of abdominal obesity and/or diabetes. The endocannabinoid actions, via the activation of CB1 receptors (CB1R), promote weight gain by increasing food intake and modulate metabolic regulation. CB1Rs are highly abundant in the brain and mediate psychotropic effects, which limits their value as a potential therapeutic target.

We have discovered a novel CB1R antagonist, GCC2680, with a potent and selective binding affinity to CB1R (IC_{50} value against rat CB1R of 0.68nM). While GCC2680 has a very potent anti-obese activity, it also has a very effective activity to control the blood glucose level in DIO mice. We also have discovered a novel CB1R antagonist, GCC2798, which was modified so that GCC2798 does not cross the blood-brain barrier, thereby reducing the risk of psychiatric side effects.

In the present study, we investigated the effect of GCC2680, a novel selective CB1R inverse agonist on the obesity and type 2 diabetes, and also compared this effect with Rimonabant, well-known CB1R inverse agonist. We also investigated the effect of GCC2798, of which BBB penetration is only 20% of Rimonabant, however, the ability of body weight reduction is as compared to Rimonabant. We also measured the anti-diabetic activities in Lep^{ob}/Lep^{ob} mice, and administration of GCC2798 (10mg/kg/day) during 4 weeks lowered serum glucose and produced improvement of HbA1c level (approximately 2%) with similar or greater potency than pioglitazone (25mg/kg/day), the beat-selling oral diabetics, while the administration of Rimonabant showed the marginal anti-diabetic activities.

We also measured various pharmacological and toxicological profiles of GCC2680 and GCC2798, and details will be presented orally.

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Small molecule drug discovery targeting DGAT1 for the treatment of metabolic disorders

곽영신

한국생명공학연구원 바이오의약연구소

Obesity and type II diabetes are intrinsically linked and considered as pandemic life-threatening diseases. DGAT1 is a key enzyme for lipid metabolism. The phenotype of DGAT1 knock-out mice validates DGAT1 as an intriguing target for the drug discovery in metabolic disease area. Multiple chemotypes were pursued to identify potent and efficacious DGAT1 inhibitors and that yielded some exciting chemistry discoveries. Important lessons were learned that would potentially impact future drug discovery programs.

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Development of Novel Therapeutic Agents for type II Diabetes using Molecular Diversity and Chemical Biology

박승범

서울대 화학부

The development of novel bioprobes can serve important role in the discovery of new therapeutic agents and study in Chemical Biology. We developed novel fluorescent glucose bioprobes to monitor the cellular uptake of glucose in physiological condition. We previously reported that Cy3-Glc-α is a novel bioprobe for bioimaging and screening for new anti-cancer agents through the efficient in vitro monitoring of glucose trafficking. As an extension of our study, we pursued the design and synthesis of a series of novel fluorescent glucose bioprobe with the variation of linker regions and fluorescent dyes, because we observed undesired aggregations of Cy3-Glc-α bioprobe at the cell surface, especially in adipose cells. This new array of fluorescent glucose bioprobes was successfully applied in the flow cytometry to monitor the global event of cellular glucose uptake. The development of novel fluorescent glucose bioprobe can provide the unique research tool for high-content screening or bioimaging which is applicable for the identification of new therapeutic agents, which regulate the glucose uptake, as a novel treatment of obesity and diabetes. Actually we discovered a small molecule AMPK activator, confirmed by western-blot analysis using phosphoAMPK antibody (T172). We also demonstrated the in vivo efficacy of our novel therapeutic agents in DIO mouse model. This compound demonstrated the actual glucose uptake in cellular system monitored by our fluorescent glucose bioprobe, which has almost identical enhancement of glucose cellular uptake by insulin.

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Current Status in the Development of Anti-diabetic Agents- Targeting ER stress and inflammation associated with lipid injury -

이명식

삼성의료원 내분비내과

Type 2 diabetes (T2D) is a metabolic disease that affects 2.8% of all age-groups worldwide, and this proportion is expected to increase to 4.4% or more than 350 million people in 2030. The two major components of the pathogenesis of T2D are insulin resistance and beta cell failure. However, the biochemical mechanisms underlying these 2 phenomena are incompletely understood. Traditionally, sulfonylurea, metformin, a-glucosidase inhibitors, and diverse forms of insulin have been used for the management of diabetes. Recently, glinides, thiazolidinedions, GLP-1 analogues or DPP-IV inhibitors were added to the inventory of antidiabetic agents based on the new mechanism of diabetes discovered during the past 15 years. However, more recent investigation revealed hitherto unknown mechanisms of the mechanism of diabetes, which include the role of ER stress and inflammation associated with lipid injury. Regarding the mechanism of lipid injury, the role of ceramide, diacylglycerol, sphingosines and phospholipids related to the insulin resistance or lipoapoptosis has been reported, which is expediting the research of the agents inhibiting their production or action. As the role of ER stress or low-grade inflammation associated with lipid injury in the pathogenesis of diabetes is uncovered, agents attenuating ER stress and inflammation are being developed as a new therapeutic modality against diabetes. Hereby, the current tendency of the developmental strategy for diabetic medicines adopted by biotech companies or laboratories is discussed.

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The Roles of the Drug Development Platform Technology on Early Discovery of Anti-Diabetic Drug

배명애, 안성훈, *송진숙, 이병회, 김민선

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신약개발은 사막에 널린 모래들 중 비밀의 문을 열 수 있는 열쇠인 딱 한 개의 모래를 찾는 일에 비유된다. 하나의 신약개발에 성공하기 위해 초기단계부터 임상단계에 이르기까지 수많은 인력과 오랜 시간, 엄청난 비용이 소요된다. 신약을 개발하는데 들어가는 비용은 8000 억에서 1 조 2000 억이며 통상 12 년이 걸린다고 한다. 이렇게 많은 비용과 시간이 소요되는 신약개발과정의 실패율과 위험부담을 최소화하기 위한 기술이 신약플랫폼기술이다.신약플랫폼기술은 다양한 신약을 만들어 낼 수 있는 기반기술로서 신약개발의 효율성 측면에서 매우 중요한 의미를 갖는다. 신약플랫폼기술은 신약개발과정 중 가장 많은 비용이 소요되는 임상단계 이전의 후보물질 발굴단계에서 약동력학・기초독성・물성분석・화학설계를 통해 신약으로의 가능성이 가장 높은 후보물질을 찾아내는 역할을 수행한다. 약동력학은 특정 약물이 체내에 투입돼 어떤 과정으로 흡수되고 어느 조직에 어떤 영향을 미친 뒤 체외로 배출되는가의 전과정을 분석하는 것이다. 기초독성은 특정약물이 가진 독성을 평가하는 것으로 심장・간 등 사람의 각 장기에 어떤 부정적인 영향과 유전적 변이를 유발하는지를 분석 평가한다. 또한 물성연구는 해당물질이 무엇에 잘 녹는지 등 물질의 물리화학적 특성자체를 분석한다. 신약플랫폼 기술은 이러한 후보물질 발군단계의 연구를 통해 글로벌 신약으로 개발 가능성이 높은 후보물질군을 확보하고 임상단계에 제공함으로써 임상단계의 실패율을 낮추고 동시에 신약개발의 위험부담을 최소화해 신약개발을 활성화시킨다. 본 심포지엄에서는 공동연구로 당뇨병 치료제 개발를 수행하면서 도출된 연구 결과들를 일부 인용 발표 하므로써 신약개발플랫폼 기술의 신약개발 초기단계에서의 역할과 중요성을 소개 하고자 한다.

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Photocarrier Dynamics in Broadband Si:Ge Nanowire Photodetectors

조문호

POSTECH

Si:Ge alloy semiconductor nanowires (NWs) offer challenging opportunities for integrated Si optoelectronics, since they potentially allow unprecedentedly strong light-matter interaction in the wavelength range of the optical communication.[1,2,3] Therein, optical and electrical properties of semiconductors at the nanometer regime manifest themselves to be strongly size-dependent, and such substantial variations have been intensively investigated as the central theme of nanoscience. Here we demonstrated a scanning photocurrent imaging technique particularly to investigate dynamics of photocarriers in individual Si:Ge NWs, by which it was spatially and spectrally resolved without ensemble average. Specifically, we show experimental demonstration of several NW optoelectronic devices, recently studied in our laboratory, where various Si:Ge NWs are functionally incorporated [4,5,6]. They will include Si:Ge NW photodetectors, intra NW p-n diodes and near-field plasmonic detectors, where the photogenerated carrier dynamics commonly size-dependent around the optical diffraction limit. References[1] Nano Lett. 6, 2679 (2006): [2] Adv. Mater. 20 1 (2008): [3] Appl. Phys. Lett. 92, 263111 (2008): [4] Nature Physics 5, 475 (2009): [5] Nano Lett. In Press (2010): [6] Submitted (2010).

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Semiconductor Nanocrystals as Color Conversion Phosphor on LED Device

장은주

삼성종합기술원 Advanced Materials

The luminescent semiconductor nanocrystals (NCs) would be an attractive candidate of color conversion phosphor material on LED device, because of NCs broad absorption range, easy color tenability and high purity compared to inorganic phosphor. For the practical application of NC to LED, NCs should be embedded in the matrix with maintaining its optical properties and enhancing stability under thermal and photo-activation condition in air. In this presentation, we will show how to stabilize NCs in host matrix homogeneously with maintaining its optical properties. We also report here on the successful integration of NC as color converting materials on blue LED.

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CIGS박막태양전지의 제조기술 동향

권세한

LG이노텍 Solar Cell Lab

에너지와 환경문제로 인하여 무공해 무한정 에너지인 태양에너지를 전기에너지로 변화시키는 태양광발전 시스템에 대한 보급이 증가되고 있다. 현재 태양전지 시장의 주종으로 이루고 있는 결정질 실리콘 태양전지는 200 ㎛ 내외의 기판을 사용하기 때문에 생산 단가를 낮추는데 한계가 있으며, 특히 실리콘 원소재의 공급 불안도 문제점으로 지적되고 있기 때문에 5 ㎛ 내외의 얇은 층만으로도 태양전지를 제조할 수 있는 박막 태양전지가 새로운 대안으로 주목받고 있다. 특히 Cu(In,Ga)Se2, CuInS2 등의 Se, S 계 화합물 박막 소재를 활용한 태양전지는 높은 광흡수 계수, 상대적으로 높은 효율, 화학적 안정성, 도시적인 미관 등으로 인하여 최근 부각되고 있다. 매년 태양전지 시장은 40% 이상 성장하고 있으며 박막 태양전지의 시장 점유율도 급상승하고 있으며, 2010 년경에는 박막 태양전지가 전체 태양전지 시장의 20% 이상을 차지하며 Se, S 계 박막 태양전지도 전체 시장의 10% 정도를 차지(13-26 억$)할 것으로 전망하고 있다. 고효율화 연구는 연구소와 학교 등에 의해 진행되고 있는데, 미국의 NREL 에서 record efficiency 를 지속적으로 갱신해서 2008 년 3 월에 19.9%의 효율을 달성함으로써 multi-crystalline Si 태양전지의 20.3%에 버금가는 특성을 보였음. 그 외에 대표적인 태양전지 연구강국인 독일과 일본에서 보다 광범위한 기초연구들이 진행되고 있다.독일의 Wurth solar 와 일본의 Showa shell 이 대표적인 CIGS 태양전지 모듈생산업체로 대면적으로 약 11%내외의 효율로 박막태양전지에서는 가장 높은 효율을 얻고 있다. 국내연구기관으로는 KIER 과 KAIST 에서 18.8%의 효율을 달성하였으며 LGIT, 삼성전자, 텔리오솔라, 대양금속에서 양산화를 위하여 Pilot line 수준의 개발이 진행되고 있다. CIGS 태양전지는 후면전극, CIGS 광흡수층, Buffer 층, 전면전극으로 구성되어 있으며, Panel 을 Modulation 공정을 진행함으로써 최종 제품으로 제조된다. 이중 광흡수층인 CIGS 박막은 약 2um 의 두께로 evaporation, sputtering&selenization, 비진공 등 다양한 공정기술로 증착된다. 본 발표에서는 CIGS 태양전지의 특성과 개발현황에

대하여 알아보고, 각 박막의 제조 방법 및 개발동향에 대하여 소개하고자 한다. 그리고 지경부지원하에 진행되고 있는 국책과제 "유리기판 CIGS 계 박막태양전지 모듈 제조기술 개발 과제"를 진행계획을 소개하고자 한다.

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A Hemispherical Electronic Eye Camera Based on Compressible Silicon Optoelectronics

고홍조

광주과학기술원 신소재공학과

The hemispherical detector geometry of a human eye enables wide field of view and low aberrations with simple imaging optics. This type of configuration is extremely difficult to achieve using established optoelectronics technologies, due to the intrinsically planar nature of fabricating process such as patterning, deposition, etching, materials growth and doping. In this study, we introduce a route to curvilinear optoelectronics and electronic eye imagers that begins with well established electronic materials and planar processing approaches to create optoelectronic systems on flat, two dimensional surfaces, in unusual designs that allow full compressibility/stretchability to large levels of strain (~50% or more). This feature enables planar layouts to be geometrically transformed (i.e. conformally wrapped) to nearly arbitrary curvilinear shapes. In the example presented here, we use a hemispherical, elastomeric transfer element to accomplish this transformation with an electrically interconnected detector array. The resulting hemispherical focal plane arrays, when combined with imaging optics and hemispherical housings, yield electronic cameras that have overall sizes and shapes comparable to the human eye. In a general sense, these methods, taken together with our theoretical analyses of their associated mechanics, provide practical routes for integrating well developed planar device technologies onto the surfaces of complex curvilinear objects, suitable for diverse applications that cannot be addressed using conventional means.

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염료 감응 태양전지의 소재 개발 동향

이지원

삼성SDI(주) 에너지랩

염료 감응 태양전지는 광전기 화학 반응에 의해 발전하는 태양전지로 소재 특성이 태양전지 성능을 많이 좌우한다. 가시광을 흡수하는 염료가 무기 나노 입자 표면에 흡착 된 광음극과 전자를 생성하는 촉매, 전자 전달을 하는 전해질로 형성된 유/무기 복합소재의 태양전지이다. 이 소재들간의 에너지 레벨이 전자 전달의 주요 추진력이 됨으로 에너지 수준을 최적화 하는 기술이 중요하다. 또한, 동종/이종 소재 계면에서 생기는 전자 손실을 최소화 하기 위한 계면처리 기술에 따라 성능이 좌우된다. 태양전지 시장의 가격 경쟁이 심화되고 있는 상황에서 염료 감응 태양전지의 조속한 상품화를 위해서 소재, 구조, 공정, 제조 장치 각 분야에서의 연구 개발이 원활이 진행되기를 기대하면서 염료 감응 태양전지 기술을 소개한다.

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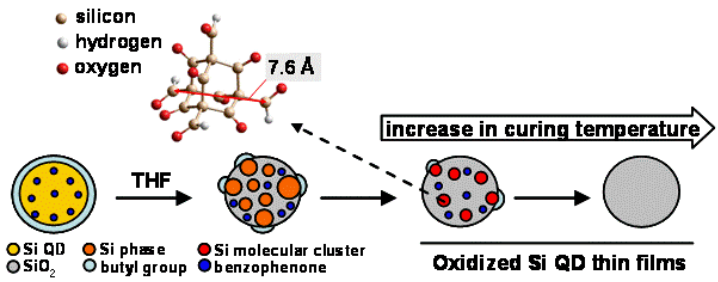
Tuning of refractive indices and optical band gaps in oxidized silicon quantum dot solids

정현담, *손홍래, 최진규, *장승현

*전남대 화학과 *조선대 화학과*

This lab has initiated compelling research into silicon quantum dot (Si QD) solids in order to utilize their synergetic benefits with quantum dot solids through fabrication of Si QD thin films. The issues of oxidation concerning the Si QD thin films were confirmed using Fourier transform infrared spectroscopy (FT-IR) and X-ray photoelectron spectroscopy (XPS). The refractive index value of the Si QD thin film at a 30 ^{o}C curing temperature was 1.61 and 1.45 at 800 ^{o}C due to complete oxidation of the Si phases. The optical band gap values of 5.49 - 5.90 eV corresponded to Si phases with diameters between 0.82 - 0.74 nm, dispersed throughout the oxidized Si QD thin films and modeled by Si molecular clusters of approximately fourteen silicon atoms. The photoluminescence (PL) energy (2.64 – 2.61 eV) in the proposed Si QD thin films likely originated from the Si=O bond terminating the Si molecular clusters.



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발표분야: 광전자 분야에서의 최신 재료화학 연구 동향
발표종류: 심포지엄, 발표일시: 목 17:00, 좌장: 조문호

Graphene Oxide를 이용한 저항 메모리 소자

최성율, *윤태현, *김종윤

*한국전자통신연구원 나노전자소자팀 *한양대 화학과*

본 연구에서는 차세대 비휘발성 메모리의 대안으로서 화학적으로 합성된 그래핀 옥사이드가 활성층으로 사용된 Al/GO/Al 적층 구조의 메모리 소자가 제작되었다. 화학적으로 합성된 그래핀 옥사이드는 Williams Hummers 가 제안한 방법으로 제조되었고 간단한 spin-coating 방법을 사용하여 하부 Al 전극 위에 대면적으로 균일하게 형성되었다. 이 소자는 I-V 측정 결과 매우 안정적인 지속성과 반복성을 지니는 이극성 저항변화 특성을 나타냈다. 저항변화 메커니즘을 규명하기 위하여 X-선 회절기(XRD), 고분해능 투과전자현미경(HRTEM), in situ X-선 광전자 분광기(In situ XPS) 등의 분석방법이 사용되었다. 산소를 함유하고 있는 그래핀 옥사이드가 Al 상부전극 증착 시 환원되면서 4~5 nm 의 상부 계면 층이 새롭게 형성되고 이와 동시에 아래에는 환원된 그래핀 막이 형성됨이 증명되었다. 이를 근거로 이 상부계면 층이 insulating barrier 로 작용하며, 외부에서 가해진 전압에 의한 산소의 이동에 따른 계면 층에 지역적 필라멘트의 생성과 소멸로 인한 저항 변화 메커니즘이 새롭게 제시되었다.

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발표분야: 재료화학분야의 최신 동향 : 신진 연구자를 중심으로
발표종류: 심포지엄, 발표일시: 금 09:20, 좌장: 한상우

Material-independent Surface Functionalization Inspired by Mussel Adhesion

이해신

KAIST 화학과

Utilizing versatile adhesion properties of marine mussels, Mytilus edulis, material-independent surface chemistry will be presented. The material-independent surface functionalization has been used in a wide variety of materials including noble metals, metal oxides, semiconductors, and synthetic organics. The presentation will cover a facile method of nanoparticle surface modification, surface PEGylation, on-surface growth of nanoparticles, surface-initiated atomic transfer radical polymerization that can apply to any types of material surfaces.

한국화학회 THE KOREAN CHEMICAL SOCIETY

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발표분야: 재료화학분야의 최신 동향 : 신진 연구자를 중심으로
발표종류: 심포지엄, 발표일시: 금 09:45, 좌장: 한상우

Surface-enhanced Raman scattering of graphene and graphene thin films using a layer-by-layer assembly method

신현석

울산과학기술대 에너지공학부

Graphene is a rapidly rising star in materials science and condensed matter physics because of its unique electronic, mechanical and thermal properties. Especially, many chemists and materials scientists are focusing on functionalization and structural analysis of graphene, graphene-based polymer composites, and graphene multilayers for transparent conducting electrodes. In this presentation, some research results will be discussed: (1) surface-enhanced Raman scattering (SERS) of graphene and (2) graphene thin films using a layer-by-layer assembly method.(1)SERS of graphene was studied for Au nanoparticles deposited on graphene by thermal evaporation. For systematic study, dependence of SERS effect on density of evaporated Au nanoparticles and excitation wavelength was first investigated to optimize experimental condition. Then, SERS spectra of single-layer and few-layer graphene were compared(2)We synthesized stable suspension of positively and negatively charged reduced graphene oxides, respectively. By exploiting the electrostatic interactions between these oppositely charged reduced graphene oxide suspensions, we made a thin film of multilayered graphene nanosheets using layer-by-layer assembly methods. The assembled graphene multilayer thin film exhibited an excellent electrical conductivity with a high optical transmittance. Furthermore, we compared the thin film fabricated by layer-by-layer assembly of reduced graphene oxides with that of graphene oxides. Lastly, we showed a light-emitting diode based on these assembled graphene multilayers as a transparent and conducting electrode.

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발표분야: 재료화학분야의 최신 동향 : 신진 연구자를 중심으로
발표종류: 심포지엄, 발표일시: 금 10:10, 좌장: 한상우

Platinum-based Metallic Nanocrystals with Shape and Composition Control for Catalytic Applications

이현주

연세대 화공생명공학과

The shape and composition of metal nanocrystals were controlled to develop catalysts with better activity and selectivity. Atomic arrangement on the surface is changed by controlling the shape of metal nanocrystal. Since most of the chemical reaction occurs via chemical adsorption of reactants on the catalyst surface, change in atomic arrangement can cause a large difference in catalytic activity and selectivity. This effect can be shown clearly in various gas-phase, solution-phase, electrocatalytic reactions. Combining with control in composition, novel fuel cell electrocatalysts with better catalytic properties have been developed in our lab.As an example of shape control, we synthesized various sizes of platinum dendritic nanoparticles, and showed that these have a superior activity, selectivity, and durability to commercial E-tek catalyst for oxygen reduction reaction and methanol oxidation. XPS results demonstrated a shift of binding energy of platinum toward negative direction, implying that electrons on dendritic nanoparticles can participate in surface reaction more easily.

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발표분야: 재료화학분야의 최신 동향 : 신진 연구자를 중심으로
발표종류: 심포지엄, 발표일시: 금 10:45, 좌장: 민달희

Water Retaining Polymer Electrolyte Membranes for Fuel Cell Applications

박문정

포항공과대 화학과

Ion-containing polymer electrolyte membranes (PEMs) have attracted considerable attention for their potential use in fuel cells. Both random copolymers wherein ion-containing groups are connected randomly to hydrophobic backbones, and block copolymers wherein ion-containing hydrophilic groups are sequestered in a fraction of the chains have been considered as PEMs. Block copolymer based PEMs are ideally suited for fundamental studies due to the fact that the size and shape of the ion conducting channels are defined by the molecular structure of the copolymer and the water content. This, in turn, enables optimization of PEMs for practical applications. In contrast, pathways for ion transport in random copolymer-based PEMs do not have a well-defined shape and size due to the polydisperse nature of the ionic domains. We establish a new systematic methodology for controlling the water retention of polymer electrolyte membranes. Block copolymer membranes comprising hydrophilic phases with widths ranging from 2 to 5 nm become wetter as the temperature of the surrounding air is increased at constant relative humidity. The widths of the moist hydrophilic phases were measured by cryogenic electron microscopy experiments performed on humid membranes. Simple calculations suggest that capillary condensation is important at these length scales. The correlation between moisture content and proton conductivity of the membranes is demonstrated.The orientation of domains in PEMs made from poly(styrenesulfonate-b-methylbutylene) copolymers (PSS-PMB) in contact with humid air is also explored. We demonstrate that at fixed composition, the sulfonation levels of the PSS-PMB copolymers play an important role in determining domain orientation.

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발표분야: 재료화학분야의 최신 동향 : 신진 연구자를 중심으로
발표종류: 심포지엄, 발표일시: 금 11:10, 좌장: 민달희

Nanostructure fabrication : top-down, bottom-up, and hybrid approaches

박인규

KAIST 기계공학과

In this talk, we discuss new approaches for nanostructure fabrication based on top-down and top-down/bottom-up hybrid methods. First, top-down nanofabrication of high density nanowire arrays and their applications in the real-time chemical sensing devices are presented. As opposed to the bottom-up counterparts, top-down approach allows facile integration and assembly of nanowires, excellent control of geometrical and electrical characteristics, and high density array configuration. This allows reliable and individually addressable nanowire array device for real-time chemical detection and active manipulation of chemical reaction in nanoscale. Second, a novel top-down/bottom-up approach based on localized bottom-up synthesis of nanowires via localized Joule heating of microheaters is introduced. This approach enables selective fabrication of nanowires and their in-situ integration on functional electronic devices. We explain the detail of this process and present a few applications of functional nanodevices made by this process in the photonic and environment sensing platforms.

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발표분야: 재료화학분야의 최신 동향 : 신진 연구자를 중심으로
발표종류: 심포지엄, 발표일시: 금 11:35, 좌장: 민달희

불균일 촉매 특성을 이용한 나노센서 연구

백정민

울산과학기술대 기계신소재공학부

One-dimensional (1-D) nanostructures of metal-oxide semiconductors are currently the subject of intense research both in order to discover fundamental science at the nanoscale as well as for their potential as sensing, catalytic, and other electronic applications. In particular, the use of nanomaterials as catalysts is perhaps the most intriguing. Reducing catalytic substances to nanometers in size greatly increases the surface area available per gram, which in turn boosts the level of catalytic activity. Furthermore, the development of MEMS microfabrication techniques and nanotechnology has significantly generated cost savings in materials used or savings in the time it takes to perform a process.Here, we describe the synthesis and properties of 1-D semiconductors (VO2 and SnO2) as novel catalytic and gas sensing materials. Of them, VO2 is an interesting material on account of its easily accessible and sharp Mott metal-insulator transition at ~ 68 °C in the bulk. Nanometer-sized liquid droplets (V2O5) produced at temperatures below the bulk melting temperature became supercooled as they grow through Ostwald ripening or coalescence and were exploited to grow nanowires without any catalyst. For potential applications, we will show the properties of VO2 and SnO2 nanowires as sensing materials of hydrogen sensor and of electronic nose, respectively. Palladium-decorated VO2 nanowire shows extraordinary sensitivity (~ 3 order-of-magnitudes) towards hydrogen, causing a significant downward shift in the Mott transition temperature. An electronic nose strategy will be described which is based on modifying the sensing properties of SnO2 nanowires in two ways: by changing their operating temperatures and by decorating some of the nanowires with metallic nanoparticles.

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발표분야: 녹색화학을 이용한 무기 및 재료 합성
발표종류: 심포지엄, 발표일시: 금 13:30, 좌장: 윤태현

Solution-Based Routes to Highly-Ordered Nanostructured Films Using Oxide Nanosheets as 2D Functional Blocks

Takayoshi Sasaki

International Center for Materials Nanoarchitechtonics(MANA), National Institute for Materials Science (NIMS), Tsukuba, Ibaraki 305-0044, Japan

We have synthesized a variety of transition metal oxide nanosheets (e.g., $Ti_{1-d}O_2$, MnO_2, $Ca_2Na_{n-3}Nb_nO_{3n+1}$ (n = 3-6), $Cs_4W_{11}O_{36}$…) through soft-chemical exfoliation of precursory layered compounds. The resulting colloidal unilamellar sheets can be utilized as 2D functional nanoscale block with enhanced optical, photochemical, electronic, and magnetic properties. We have applied solution-based techniques such as Langmuir-Blodgett deposition and sequential adsorption procedure to assemble these oxide nanosheets layer-by-layer into highly ordered multilayer and superlattice-like films. Selection of nanosheets and precise nanoarchitectural design of the assemblies can lead to useful functionalities such as efficient photovoltaic conversion, magneto-optical response to UV light and high dielectric properties at a nanometer scale.

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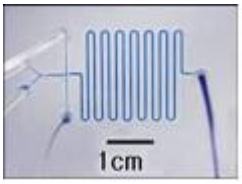
발표분야: 녹색화학을 이용한 무기 및 재료 합성
발표종류: 심포지엄, 발표일시: 금 14:00, 좌장: 윤태현

Lab-on-a-Chip Systems for Microchemical Synthetic Applications

김동표

충남대 공업화학과

Microreaction at has been successfully used in analytical chemistry and bio-applications. The microfluidic device has been generally fabricated with durable glass, Si and metal by expensive MEMS techniques, alternatively with facile PDMS and PMMA by soft lithography techniques. By adopting the advantages of both plastic and glass categories, it is desirable to fabricate the novel polymer based lab-on-a-chip microfluidics with high stability by facile process. At first, we report farbication of novel polymer based lab-on-a-chip microfluidics with high stability by facile process, as well as the microchemical syntheses as device applications. The organic solvent resistant lab-on-a-chip systems from Si-based polymers, including inner-surface coated PDMS microchannels and a flexible polyimide film microreactor were used for different catalytic and enzymatic reactions. And PDMS microfluidics with unique design were also useful for cell-free protein synthesis and gas-liquid oxidative Heck reaction with high selectivity. In addition, we introduce lab on a chip systems with built-in microstructures embedded in the microchannels. These results demonstrate that the built-in microchemical chip definitely enhance the uniqueness and performance of microfluidics.



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발표분야: 녹색화학을 이용한 무기 및 재료 합성
발표종류: 심포지엄, 발표일시: 금 14:30, 좌장: 윤태현

Green Nanotechnology Based on Ionic Liquids for Applications into Energy and Biosensor Devices

박호석

경희대 화학공학과

The concept of 'green nanotechnology' is of prime importance in terms of reducing impacts on human health and the environment for practical applications. Ionic liquids (ILs), which have been attracted as green solvents early, extend their applicative fields into the nanotechnology due to the unique, tailorable, and remarkable physicochemical properties and multi-functions. In this work, ILs serve as the hierarchical multifunctional material in terms of acting as template and solvent agents in the design and fabrication of functional nanomaterials, assembling and positioning nano-objects, and conducting ions or interacting with target materials in the process of device operation. Therefore, ILs can "design" various nanomaterials, i.e. inorganic nanocrystals, IL/inorganic nanohybrids, and carbon nanotube (CNT)-based nanocomposites, and "function" for applications into electrochemical devices, separation, and photocatalysis.Thus far, we have developed two green nanotechnologies based on ILs, i.e. ionothermal process and IL-assisted sonochemical method (ILASM), to fabricate functional nanomaterials. The gallery of nanomaterials fabricated by and/or composed of ILs was inorganic nanocrystals, IL/inorganic nanohybrids, and CNT/IL/NP nanocomposites. An ionothermal synthetic method is a powerful route to fabricate the shape-controlled inorganic nanocrystals (γ-Al2O3, α-Fe2O3) and IL/inorganic nanohybrids (IL/γ-AlOOH, IL/β-FeOOH), having advantages over conventional solution syntheses in points of eliminating the complications associated with high hydrothermal pressures in a sealed autoclave and avoiding the post-addition of organic solvents. An ILASM offers a versatile, facile, and rapid way to fabricate emerging CNT-based nanocomposites by means of combining supramolecular chemistry between ILs and CNTs for the dispersion and functionalization of CNTs with sonochemistry for the in-situ synthesis and decoration of various nanoparticles (Pt, Pd, Au, Ag, Sn, Fe, ZnO, CdTe). IL-based green nanotechnology suggested herein opens new pathway toward the design and fabrication of functional nanomaterials and their applications into conventional and emerging technologies.

대한화학회
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발표종류: 심포지엄, 발표일시: 금 15:10, 좌장: 박강현

울산 녹색화학 지향하는 기후변화 협약대응 기업지원사업

강선희

(재)울산테크노파크 정밀화학사업단

대한민국 정부에서 2009 년 온실가스 배출에 관한 목표량을 산정하여 발표하였고, 이는 정부의 적극적인 감축 목표량을 산정하여 추진하려는 강한 의지를 보인다. 기후변화에 대한 발 빠른 대응과 협약 대응책으로 기업체의 대응기반 마련, 자발적 온실가스 감축활동 필요한 실정이다. 산업단지가 많이 형성되어 있는 울산 내 중소·중견 기업체들의 에너지 효율 향상 및 CO2 절감 위한 지역 거점 지원 기관 필요하고, 이에 울산테크노파크(정밀화학사업단)이 한발 앞서 기후변화 협약대응 기업지원사업을 추진하고 있다.(재)울산테크노파크 정밀화학사업단 (단장 남두현) 에서는 지역전략산업진흥사업(사업명: 기후변화협약 대응 기업지원사업)의 일환으로 기업체의 생산 활동 전 과정의 에너지 효율을 향상시켜 근원적으로 울산지역 내 기업체가 이에 대한 기후변화협약 대응책으로 기업체의 대응기반 마련, 공정진단을 통한 에너지 절감 및 온실가스 배출 저감 컨설팅, 온실가스감축 활동, 환경라벨링 인증 및 인벤토리(Inventory) 구축을 지원하는 사업을 진행 중이다. 2009 년 기후변화협약 대응 기업지원사업을 통해 연간 약 21 억원 규모의 경제적 효과를 얻었으며, 온실가스 이산화탄소(CO2) 16,065 ton/yr 절감하였다.또한, 울산정밀화학사업단은 세계 최대 과학학회인 미 화학학회(ACS)의 산하 연구소인 "녹색화학연구소 (GCI)"에 한국지부로 가입하여, 녹색화학 관련 기술 및 교육 분야의 이용 및 정보교류, 국제 세미나 개최 및 기술자문, 선진기술 및 정보 공유에 관하여 협력하고 있으며, 캐나다 Eco-efficiency 센터, 독일 BASF(최대 글로벌 화학기업)-Sustainable center 와 국제 공동협력 관계를 통하여 녹색 소재 기술 발굴 및 이전을 통하여 맞춤형 녹색화학 신산업 창출 기회 마련 및 국제 경쟁력 강화에 핵심 앵커 역할을 담당하고 있다.

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장소: 송도컨벤시아

발표코드: **금20I5심**

발표분야: 녹색화학을 이용한 무기 및 재료 합성

발표종류: 심포지엄, 발표일시: 금 15:40, 좌장: 박강현

Engineering Macromolecular Self-Assembly for Applications in NanoBiotechnology

김병수

울산과학기술대 친환경에너지공학부

Block copolymers have been the focus of much research interest during last 30 years due to their unique self-assembly behavior. Combined with their potentials of self-assembly at nanometer scale and the progress of nano- and biotechnology, block copolymers are increasingly finding their applications as tools for nanofabrication, templates for other nanomaterials, structural components in hybrid materials and nanocomposites, and as nanocarrier for drug delivery. In this presentation, I will describe the research efforts to address the challenges present in nano- and biotechnology by taking advantages of the self-assembled block copolymer nanostructures. The first part of the talk will introduce the block copolymer based non-covalent, topological surface modification method for inorganic nanoparticles as a general means to protect the nanoparticles and to conjugate biological molecules. In particular, magnetic and semiconducting nanoparticles are integrated with the amphiphilic block copolymer micelle and used as recyclable enzyme supports and biological labels for extreme physiological conditions. The second part of the talk will briefly illustrate the exploitation of block copolymer as a nanometer sized vehicle to deliver hydrophobic therapeutics from the surfaces. Layer-by-layer self-assembly method was particularly employed for fabricating multilayer thin films with controllable structure and composition. This method would provide a general means to deliver active therapeutics in biomedical applications for therapeutic surface coatings and also for tissue engineering scaffold.

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발표분야: 녹색화학을 이용한 무기 및 재료 합성
발표종류: 심포지엄, 발표일시: 금 16:10, 좌장: 박강현

일산화탄소 상온 제거용 다공성 촉매 실용화 기술

이철위

한국화학연구원 그린화학연구단

맹독성 "일산화탄소를 실온에서 제거하는 촉매 연구"가 학문적으로나 상업적으로 수많이 시도되고 있으나, 현재까지 성능, 내구성 및 가격을 동시에 만족하는 촉매가 개발되어 상용화된 사례는 흔하지 않다. 잘 알려진 알루미나, 제올라이트, 활성탄 등의 담체에 귀금속이 담지된 촉매는 가격이 비싸며, 초기성능은 우수하지만 수분이 공존하게 되면 성능이 급격히 감소하여 내구성이 결여되어 상용화되지 못하고 있다. 이러한 문제를 해결하기 위한 핵심기술은 활성금속 원료를 나노분산 시키는 기술 및 반응 중에 항상 공존하는 수증기의 방해효과를 최소화하기 위하여 소수성이며 나노 크기의 세공을 갖는 표면적이 큰 (~500m2/g) 담체의 생산 기술 그리고 소재의 재생/재활용기술을 확보하는 것인데 이로부터 수증기 및 여타 가스가 공존하는 조건에서도 장시간 일산화탄소 제거가 가능하게 되었다. 본 연구에서는 일산화탄소를 상온에서 제거할 수 있는 국내에서 성공적으로 실용화된 촉매기술을 소개한다.

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발표종류: 심포지엄, 발표일시: 금 13:30, 좌장: 이충균

Boosting up Electron Transfer: for Next Generation Energy and Bio technologies

송현곤

UNIST (울산과학기술대) 친환경에너지공학부

Four different strategies could be considered to enhance electron transfer of an electrochemical system consisting of electrodes and electrolyte including molecules of interest: (1) to optimize porous structure of electrodes, (2) to add functionality such as electroactivity and electrochromism onto the body of electrodes, (3) to modify the interface between electrodes and electrolyte and (4) to use mediators shuttling between electrodes and target molecules. In this talk, several interesting ideas related to forementioned strategies are introduced to enhance the electrochemical systems that can be used for energy and bio technologies. (1)“Electrochemical porosimetry” reveals porous structure of electrodes that ions in electrolyte actually feel. (2)The method of “incorporation of functional dopants into conducting polymers” is introduced as the strategy to add functionality to electrodes or materials for biofuel cells, flexible polymer batteries, electrochromic devices and even biomaterials for nerve regeneration. (3)Selective electrochemical detection: Different molecules of an identical redox potential can be identified by modifying the surface of electrodes.(4)Nanoparticles can be used as a wireless booster or a mediator to enhance productivity of enzymatic conversion.

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발표종류: 심포지엄, 발표일시: 금 14:05, 좌장: 이충균

The Way of Roll-to-Roll Printed 13.56 MHz RFID Tags: Demonstration of All Printed 13.56 MHz 4 bit RFID Tags

조규진

순천대 화학공학과

A ubiquitous low-cost tag society will be fully realized when people can track all items with a radio frequency identification (RFID) system instead of the current barcode system. That means all goods need to have their own RFID tags. To place RFID tags on all goods, the most important factor is the cost of the tags that optimally less than one cent (0.01$). To dramatically reduce the cost of current RFID tags, a roll-to-roll (R2R) inline printing process to print all the units of the passive RFID tag, such as the antenna and transponder, has been considered as an alternative to the current Si-based technology. During the last decade, developing RFID tags using organic semiconductors with a photolithographic process has been demonstrated, however, there has been no report of production of tags that had been fully printed and R2R printable. The major reasons for the delay in developing all-printed tags originates from the lack of technology for producing an all-printed plastic rectifier that can provide at least 10 volts DC from 13.56 MHz RFID reader, and an all printed-plastic logic circuits that can generate 96 bit of signals to read a 96 bit RFID tag in a second under the DC power provided from the rectifier. Here we describe a way to achieve this goal using plastic foil substrates, and as a consequence of pursuing the ways, R2R printed 13.56 MHz operated 4 bit RFID tags and RF Logos will be demonstrated.

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Engineering Nano-composite Oxide SOFC electrodes for Efficient Oxidation of Methane

김건태

울산과학기술대 친환경에너지공학부

Fuel cells are the high efficient and environmentally friendly energy conversion devices due to the conversion of chemical energy directly into electrical energy. Solid oxide fuel cell(SOFC) is consist of only ceramics, making thermally robust and simple design. One of the main advantages of SOFC is enable to use any combustible species as fuels such as various hydrocarbons since the oxygen ainon (O2-) is mobile species. In this study, ceramic anodes for solid oxide fuel cells (SOFCs) were prepared by aqueous impregnation of nitrate salts to produce composites with 45 wt % La0.8Sr0.2Cr0.5Mn0.5O3 (LSCM) and 40 wt% La0.8Sr0.2Sc0.2Mn0.8O3 (LSSM) in a 65% porous yttria-stabilized zirconia YSZ scaffold. Scanning electron micrographs indicate that the LSCM coats the YSZ pores following calcination at 1473 K in air, the LSCM coating, however, becomes porous upon reduction, creating more the Triple Phase Boundary (TPB) where electrochemical reaction occurs. The LSCM and LSSM composites produced in this manner exhibit conductivities at 973 K of approximately 1 S/cm in air and 0.1 S/cm in humidified H2, and 5 S/cm in air and 0.38 S/cm in humidified H2, respectively. A SOFC with a composite anode composed of 45 wt % LSCM, 0.5 wt % Pd, and 5 wt % ceria exhibited maximum power densities at 1073 K of 1.1 and 0.71 W cm−2 in humidified 3% H2O H2 and methane, respectively.

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발표종류: 심포지엄, 발표일시: 금 15:30, 좌장: 김혁한

Molecular Orientation of Endohedral Metallofullerene Molecules demonstrated by Scanning Tunneling Microscopy

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Intramolecular structures of endohedral metallofullerenes (M@C82s) have been observed by scanning tunneling microscopy. In our previous report (NANO LETTERS, 2005, 5, 1057), we studied the single molecular orientation switching of the endohedral metallofullerene by using scanning tunneling microscopy. Here, we identified the molecular orientation of Lu@C82 by comparing molecular-resolution STM images of Lu@C82 molecules with molecular orbitals of Lu@C82 calculated by density functional theory. Spatial mapping of the differential conductance on individual Lu@C82 molecules revealed that the local conductivity within a molecule became large around the Lu atom at a negative sample bias voltage. We also demonstrated changes in the molecular orientation of Lu@C82 by applying a high electric field. We believe that these results have obvious relevance for single-molecule switching of endohedral metallofullerenes.

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Molecular Memory using Redox-active Materials

이효영, 민미숙, 이은교, CUIPENG, 황은희, *윤여홍, *이혜미, 김지연, 김창화

*성균관대 화학과 *성균관대 에너지과학과*

Several researchers have demonstrated possible voltage-driven molecular memory devices possessing the advantages of fast response time and highly dense circuits over a photo-driven circuit, using a molecular monolayer for metal-molecule-metal (MMM) devices. Recently, in the development of the voltage-driven molecular memory devices, various redox-active organic molecules had been proposed with a help of cyclic voltammetry (CV) that provides a clue of possible candidates for molecular memory materials. Herein, we present the design, synthesis, and characterization of redox-active molecuales, and the novel fabrication of molecular monolayer devices. Finally, we like to introduce organic dye and organic radical materials for a possible switch and memory.

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발표분야: KCS School 정보전자 산업에서 화학 소재
발표종류: 심포지엄, 발표일시: 목 13:30, 좌장: 정택모

Understanding Oxide TFT

박상희

한국전자통신연구원

차세대 디스플레이는 초고화질/현실성을 추구하는 방향과 사용자의 편의성을 중시하는 두가지 방향으로 발전할 것으로 예상되며 이러한 제품의 개발을 위해서 고이동도 산화물 TFT 연구가 최근 3,4 년 사이에 급격하게 진행되고 있다. 본 발표는 산화물 TFT 의 개발 현황, 특성 향상을 위한 이슈 및 특성 향상을 위해 산화물 반도체 소재의 unique 한 물성의 이해 및 산화물 TFT 의 background 에 대해 설명한다. 또한, 최근에 많은 연구가 진행되고 있는 solution processed 산화물 TFT 개발 현황에 대해 요약한다.

THE KOREAN CHEMICAL SOCIETY

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발표종류: 심포지엄, 발표일시: 목 14:10, 좌장: 정택모

White light-emitting diode lamps using (oxy-)nitride phosphor

김창해

한국화학연구원 화학소재연구단

The blue-chip-based white light-emitting diode (LED) lamps will come in useful to the solid state lighting. Moreover, for art objects, shop window displays, and medical applications, color rendering indices of LED lamps are needed to be improved for such applications. we selected and prepared bluish-green BaSi2O2N2:Eu2+, green SrSi2O2N2: Eu2+, orange BaSi2O2N2:Eu2+, red CaAlSiN3:Eu phosphor, and then made several white LED lamps using these four oxyntride/nitride phosphors and the blue LED chip of 1 ㎟. The luminous efficacy, the correlated color temperature (CCT) and the color rendering index of the white LED lamp are measured. The high color rendering index Ra value is above 90 at the color temperature of 6,632K. It means that it is possible to realize a high color rendering white LED lamp using blue LED chip instead of UV LED chip. The luminous efficacies of white LED lamps are 50–56 lm/W under a forward-bias current of 350 mA at room temperature. It is good enough for high color rendering white LED.

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반도체 Precursor의 개발 동향

유승호

비엔아이테크

정보전자 소자 관련하여 고유전율 게이트 절연막, 저유전체막, 캐패시터 유전체막 금속배선막, 확산방지막 등 각종 기능 재료들이 화학증착법으로 만들어져 왔으며 이를 위하여 다양한 화학전구체가 활용되어 왔다. 화학증착기술을 이용하여 소자를 구현하기 위하여는 무엇보다도 사용하는 전구체의 개발과 그 특성의 평가가 선행되어야 한다. 반도체 공정의 발전과 함께 그 중요성이 더욱 커지고 있는 화학전구체의 개발동향을 알아본다.

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발표종류: 심포지엄, 발표일시: 목 15:40, 좌장: 홍인석

디스플레이용 고분자 필름 및 소재 (폴리이미드를 중심으로)

원종찬

한국화학연구원 화학소재연구단 정보전자폴리머연구센터

현대인의 일상생활에서는 노트북, 핸드폰, LCD 카메라, 네비게이터 등 각종 이동 통신 수단들이 생활의 구석구석에서 활용되고 PDP, LCD, OLED 등 평판디스플레이가 CRT TV 를 대체하고 있으며 앞으로는 e-book, 유연성 디스플레이 및 3D 매체의 환경으로 진화할 것으로 예상된다. 본 강연에서는 이들 디스플레이를 구성하고 있는 소재들 중에서 LCD 디스플레이를 구성하는 판넬, 모듈 및 BLU 에 사용되는 다양한 고분자 필름 및 소재를 소개하고, 이들 소재 중 초기에는 군사 및 항공우주용으로 연구 개발되었지만 현재는 정보전자용 소재로써 다양하게 사용되고 있는 폴리이미드의 구조, 기능, 용도 및 연구동향 등을 소개하고자 한다.

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발표코드: **목22K5심**
발표분야: KCS School 정보전자 산업에서 화학 소재
발표종류: 심포지엄, 발표일시: 목 16:20, 좌장: 홍인석

유기전자소자용 반도체 및 절연체 소재

표승문

건국대

흔히 플라스틱이라고 불리는 고분자 소재는 금속이나 세라믹 소재에 비하여 가볍고 가공이 상대적으로 용이한 장점을 가지고 있어 지난 수십 년간 인류의 생활방식에 많은 변화를 가져왔다. 일상생활의 필수품으로부터 자동차와 항공 부품, IT, BT, NT 등의 분야에도 응용되고 있다. 최근 들어 고분자 및 유기물을 이용한 전자소자에 관한 연구가 활발히 이루어지고 있다. 이는 고분자 및 유기물의 물리/화학/전기적 특성들이 그들의 화학 구조 및 공정에 따라 비교적 용이하게 제어될 수 있기 때문이다. 본 강의에서는 대표적인 고분자/유기물 반도체 및 절연체의 소개, 이들의 전기적 특성 및 이를 이용한 대표적인 유기전자소자를 포괄적으로 소개하고자 한다.

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발표분야: KCS School 정보전자 산업에서 화학 소재
발표종류: 심포지엄, 발표일시: 목 17:00, 좌장: 홍인석

Current Status of Organic Semiconducting Materials for Organic Photovoltaic Cells

윤성철

한국화학연구원 화학소재연구단

지난 몇 년 동안 유기태양전지의 에너지 변환효율은 비약적으로 발전하여 왔다. 1990 년대 초 1%대의 에너지변환효율을 갖는 벌크헤테로정션 타입의 유기태양전지가 소개된 이래, 지속적인 재료 및 소자제작 기술 개발을 통해 2009 년 말에는 미국 Solarmer 사에서 7.9%의 에너지변환효율을 달성하였다. 기존 무기계 또는 염료감응형 태양전지와 비교하여 저온 용액공정을 통해 쉽게 저가/대면적화가 가능한 장점으로 인해 상업화에 대한 가능성이 높아지고 있는 상황이다. 유기태양전지 소자는 ITO 등의 투명전극 위에 p-형 및 n-형 유기반도체 재료를 혼합하여 스핀코팅 또는 인쇄법을 통해 광활성층을 형성하고 전극을 증착하는 방법으로 손쉽게 제작할 수 있어, 향후 플렉시블 기판을 이용하여 롤투롤 연속공정을 적용하게 되면 획기적인 원가절감이 가능한 차세대 태양전지이다. 본 발표에서는 유기태양전지관련 최근 연구동향, 광활성층재료용 유기반도체 재료 및 소자제작을 위한 인쇄공정 적용 사례 등을 소개하고 상업화의 가능성을 타진하고자 한다.

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발표분야: 교사양성대학의 화학교육에 대한 초점
발표종류: 심포지엄, 발표일시: 목 14:00, 좌장: 박현주

교사양성대학의 화학교육 방안 모색의 의미

백성혜

한국교원대 화학교육과

비사범대학과 차별화된 교사양성대학으로서 사범대학의 교육에 대한 방향 모색을 해 보고자 한다. 특히 교육학, 교과내용학, 교과교육학 등으로 분리된 채 운영되는 사범대학의 교사양성 교육과정의 비효율성에 대해 논의하고, 교수에 필요한 실천적 지식으로써의 Subject Matter Knowledge(SMK)의 필요성에 대해 고찰해 볼 예정이다. 이러한 논의를 통해 사범대학의 고유한 기능이라고 할 수 있는 교사 양성 교육의 정체성을 보다 공고히 하여야 교사 양성을 목표로 하지 않는 비사범대학 교육과정과 차별화가 가능할 것이며, 궁극적으로 교사의 교수전문성을 인정받을 수 있게 될 것이다. 현재까지사범대학과 자연대학 등 비사범대학에서 교사양성을 위해 운영하는 교육과정을 보면, 학점 수 등에서 다소 차이가 있을 뿐, 궁극적으로 다루는 내용의 질적 차이를 찾아보기 어렵다. 따라서 교과교육학의 학점이나, 교육실습 기간과 횟수를 늘림으로써 양적인 차별화는 큰 의미가 없다고 생각하며, 이보다는 실제 교육 현장에서 필요한 교사 전문성과 연결되는 실천적 지식의 발달을 위한 교육과정의 질적 변화가 요구된다.

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발표분야: 교사양성대학의 화학교육에 대한 초점
발표종류: 심포지엄, 발표일시: 목 14:20, 좌장: 박현주

교사양성대학의 무기화학교육에 대한 초점

김봉곤

경상대 화학교육과

우수한 화학교사가 되려면 일반 교육학 지식(pedagogical knowledge), 화학 내용학 지식(chemistry contents knowledge) 및 교과교육학 지식(pedagogical contents knowledge, PCK)을 갖추어야 하지만, 실천적 지식으로 화학의 개념적 지식과 절차적 지식이 무엇보다 중요하다. 여기서 교원양성대학의 화학교육과에서 교과내용학 영역으로 무기화학 분야 교육의 정상화 방안을 논의하고자 한다. 화학자를 양성하는 비사범대학과 달리 중등화학교사를 양성하는 사범대학 화학교육과에서 요구되는 전공 내용학의 범위와 수준에 대한 교수 및 현장교사들의 논의는 사범대학의 무기화학교육의 정상화를 위해서 매우 중요하다. 이러한 논의를 위해서 첫째, 중등학교 화학의 교과내용을 바탕으로 무기화학분야에서 요구되는 내용영역 및 교원양성대학의 무기화학 교수요목을 비교하고, 둘째 교원임용시험에서 무기화학분야의 문항을 출제범위와 수준을 분석하며, 셋째 임용시험에 대한 사범대학에서 무기화학 강의담당 교수 및 현장교사들의 인식을 분석하였다. 이러한 분석결과를 바탕으로 교원임용교사에서 무기화학분야의 출제 범위와 수준에 대한 표준화 방안을 제안함으로써 교사 양성 교육의 정체성을 확보하고 궁극적으로 화학교사의 교수전문성을 함양할 수 방안을 제시할 것이다.

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발표분야: 교사양성대학의 화학교육에 대한 초점
발표종류: 심포지엄, 발표일시: 목 14:40, 좌장: 박현주

교사양성대학의 분석화학교육에 대한 초점

김인환

대구대 화학교육과

중등교사 임용후보자 선정 경쟁시험 제도 방식이 제 1 차 5 지 선다형 객관식 및 제 2 차 논술형 필기시험, 제 3 차 교직적성 심층면접과 수업능력 및 실험실기능력 평가 등의 3 단계로 변경되고, 2009 학년도 및 2010 학년도 경쟁시험 2 회에 걸쳐 실시되었다. 여기에서는 분석화학 분야에 대한 평가 영역에 따른 평가 내용 요소를 중심으로 사범대학 화학교육과 교육과정에서의 분석화학 관련 전공 교과목에서 다루어지는 내용에 관하여 논의하고자 한다. 이를 토대로 자연대학 화학과의 교육과정과 차별화된 사범대학의 분석화학 관련 교과목 교육내용을 연구하였다. 또한 최근 중등임용시험을 거쳐 임용된 현직 화학교사들의 분석화학 임용시험문제와 관련된 견해를 청취하여 중등교육 현장에서의 유능한 화학교사 양성에 필요한 핵심요소를 파악하였다. 이를 통하여 화학 지도에 대한 능력이 뛰어난 화학교사 양성에 따른 대안을 모색하고자 하였다.

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발표분야: 교사양성대학의 화학교육에 대한 초점
발표종류: 심포지엄, 발표일시: 목 15:20, 좌장: 백성혜

교사양성대학의 물리화학교육에 대한 초점

김도환

대구대 화학교육과

중등교원 임용후보자 선정 시험 방식이 1 차 5 지택일형 객관식 및 2 차 논술형, 3 차 수업 및 실험 시연 등으로 변경되고, 2 차례 시행되었다. 본 발표는 물리화학 분야에 대한 평가 영역 및 평가 내용 요소를 중심으로 사범대학 화학 교육과의 교육 과정에서의 물리화학 전공 수업에서 다루어지는 내용에 대해 논의하였다. 이를 위하여 기존 사범대학에서 사용되는 물리화학 교재에 대한 비교 분석을 통해 공통 요소를 추출하였다.

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발표분야: 교사양성대학의 화학교육에 대한 초점
발표종류: 심포지엄, 발표일시: 목 15:40, 좌장: 백성혜

교사양성대학의 유기화학교육에 대한 촛점

정규관

전북대 과학교육학부

중등교사임용시험이 2 단계 전형에서 현행 3 단계 전형으로 바뀐지가 두 해가 지났다. 시험전형을 바꾼 주된 이유가 교직 적격자 선발기능을 강화하기 위해서라고 제시하고 있다. 개편된 화학교사선발 임용시험에서 과거와 비교해서 유기화학에 대한 출제 경향은 어떻게 변화되어 왔는지, 그리고 시험은 개편된 평가틀에 따라서 출제되고 있는지, 출제의 방향은 개편된 평가영역과 상세화된 평가 내용 요소 내에서 출제되고 있는지를 분석해본다.

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발표분야: 교사양성대학의 화학교육에 대한 초점
발표종류: 심포지엄, 발표일시: 목 16:00, 좌장: 백성혜

교사양성대학의 화학교육에 대한 초점

박현주

조선대 과학교육학부

화학교사 임용시험의 화학교육 관련 분야를 살펴보면, 학교 현장에서 학생을 위한 교수/학습 활동을 위하여 화학교사로서 갖추어야 할 이론과 이를 수업 상황에서 적용하고 실행할 수 있는 능력, 특정 한 영역의 과학(화학)교육학적 지식보다는 다양한 영역을 동시에 어우를 수 있는 통합적이고 총체적인 능력, 교육학적 지식과 과학 지식과 더불어, 과학(화학)교육적 PCK(pedagogical content knowledge)를 측정하고 있다. 이러한 능력들이 화학교사의 전문성 평가를 위한 분야라고 전제할때, 교사양성대학의 화학교육은 어떻게 진행되고 있는가를 살펴보고자 한다. 즉, 교사양성대학에서 현재 이루어지고 있는 화학교사의 전문성 개발을 위한 교과과정을 살펴본 후, 교과과정과 교사임용시험과의 연관성에 대하여 논의하고자 한다.

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장소: 송도컨벤시아
발표코드: **목24B1심**
발표분야: Royal Society of Chemistry 심포지움
발표종류: 심포지엄, 발표일시: 목 14:00, 좌장: 장종산

Mechanochemistry – using grinding to avoid the use of solvents

Stuart James

Queen's University Belfast

One of the most striking aspects of using grinding to induce chemical reactions (mechanochemistry) is that it can often be done with solid reagents and no solvent. It therefore has the potential to provide greener synthetic methods. However, the scope and fundamental aspects of the technique still require much investigation.Aspects of this research in our group will be presented, centred around the formation of metal complexes including microporous metal-organic frameworks. Collaborative work in other types of synthesis will also be presented.

THE KOREAN CHEMICAL SOCIETY

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발표코드: **목24B2심**
발표분야: Royal Society of Chemistry 심포지움
발표종류: 심포지엄, 발표일시: 목 14:30, 좌장: 장종산

Ionic Nanomaterials and Their Applications in Catalysis

이상기

이화여대 화학/나노과학과

The integration of chemical units of pre-designed chemical function such as recognition sites, redox groups, or chromophore units, may yield hybrid systems combining the unique features of nano-sized materials with the tailored properties of the molecular or macromolecular coatings. Hybridization of organic molecules bearing characteristic properties with nano-sized materials such as nanoparticles, carbon nanotubes, and nanodiamonds is an especially attractive target, as it can improve the physiochemical properties of the nanosized materials, and create new materials possessing the unique properties, which are not appeared in the parent materials. In this context, ionic liquids could be attractive target molecules. Ionic Liquids (ILs) are organic molten salts and are made up of two components i.e. the anion and cation. As both anion and cation can be varied, these materials can be designed for a particular set of properties such as solubility, density, refractive index, and viscosity. The favorable and readily tunable physicochemical properties of ILs, especially imidazolium cation-based ILs have led to intense interest in these materials as alternatives to conventional organic solvents in a range of synthesis, catalysis, electrochemistry and liquid-liquid extractions. However, no extensive studies on the hybridization of ionic liquids with nanomaterials have been made. Recently, we have demonstrated that the tunable property of ILs can be transposed onto the self-assemble monolayers formed with thiol- and trialkoxysilane-functionalized imidazolium salts onto the Au and SiO2 surfaces. It has been also found that through the surface-functionalization of nano-materials with imidazolium salts, the solubility of the ionic nanosized materials can be controlled. These ionic nano-materials could have a potential for variety of applications such as support materials for nanocatalysts. In this seminar, our recent studies on the ionic liquid-nano hybrid will be presented.

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장소: 송도컨벤시아
발표코드: **목24B3심**
발표분야: Royal Society of Chemistry 심포지움
발표종류: 심포지엄, 발표일시: 목 15:00, 좌장: 장종산

Ionic liquids in-vacuo

Pete Licence

The University of Nottingham

Ionic liquids are, in general, organic based salts with melting points below 100 °C. This lecture describes a series of completely new experiments that are only made possible because these liquids are composed entirely of ions and consequently have almost zero vapour pressure, i.e. they do not evaporate even under vacuum. We have recognised that this lack of volatility allows ionic liquids to be used in a whole range of analytical instruments that require high vacuum for their operation. We have obtained high quality X-ray photoelectron spectroscopy (XPS) data of the pure liquids as well as the liquids doped with simple metal salts. XPS provides information about the electronic structure of different elements within a compound and has sufficient sensitivity to distinguish between atoms of the same element situated in chemically distinct environments, (see fig, left). Under our analysis conditions, liquid RTILs emit a surprisingly good photoelectron flux; hence, excellent XPS data can be obtained in a very short collection time (> 5 mins). Furthermore, since the RTIL is electrically conducting, none of the problems associated with differential charging are encountered, and charge neutralisation is not required. RTILs appear to be very stable during exposure to the X-ray source, we have observed no evidence of either out-gassing, after initial pump-down, or beam damage to the sample.The lecture will also give an overview of other activities from our group including the investigation of spectroelectrochemistry at UHV (EC-XPS) and the determination of thermodynamic data, including (ΔH_{vap}), using more traditional surface techniques including temperature programmed desorption (TPS) and line of sight mass spectrometry (LOSMS).

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Chemical properties of mass-selected clusters and nanoparticles in various environments

김영독

성균관대

Clusters consisting of less than ~ 100 atoms can show physical and chemical properties, which are significantly different from those of larger particles and bulk counterparts. Properties of clusters can be much altered with every additional atom. In this talk, interactions between oxygen and mass-selected clusters in the gas phase as well as deposited on surfaces will be discussed. For free Au clusters anions, only even numbered-clusters consisting of less than 21 atoms were found to be active for the O2 chemisorption at room temperature. A similar even-odd alteration of the O2 chemisorption reactivity was observed for Ag cluster anions. Photoemission spectroscopy could provide direct evidence on non-dissociative chemisorption of O2 on some coinage metal cluster anions. When the mass-selected Au clusters are deposited on solid surfaces, the significant size-selectivity of chemical properties can still be found. Au clusters with same sizes deposited on SiO2 and HOPG show dissimilar chemical properties, implying that deposition of mass-selected clusters on various substrates can provide a deeper insight into metal-support interactions.Nanoparticles consisting of more than several hundreds atoms behave differently from the respective bulk crystals. Oxidation and reduction behaviors of Au and Ag nanoparticles supported by silica and HOPG are sensitive to the particle size. Experiments using X-ray Photoelectron Spectroscopy can shed some light onto the size selectivity of chemical properties of nanoparticles smaller than ~ 10 nanometers in diameter. Oxide nanoparticles can be prepared using Atomic Layer Deposition (ALD). Size-dependent change in the photocatalytic activity of TiO2 nanostructures supported by C fiber will also be presented.

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발표종류: 심포지엄, 발표일시: 목 16:20, 좌장: 이상기

Towards more sustainable production of pharmaceuticals and fine chemicals

Andy Wells

Chemical Sciences, AstraZeneca

In an arena of constantly increasing demand along with finite and dwindling supplies of natural resources, society needs to move towards a more sustainable way of life if the balance of maintaining human health and wellbeing whilst preserving the environment and diversity is to be achieved. Over the past 10 years or more a number of academic and industrial groups have focused on the identification and application of greener chemistry and engineering solutions This presentation will look at some of the drivers and changes to enable the chemistry – using industries to become more sustainable. This will include synthetic strategy, chemo-bio and organo-catalysis, use of solvents and alternatives, process intensification and the application of life cycle assessment to guide the development of greener technologies.

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발표분야: Royal Society of Chemistry 심포지움
발표종류: 심포지엄, 발표일시: 목 16:50, 좌장: 이상기

Microwave Synthesis of Nanoporous Materials: Encounter of Microwave with Materials Chemistry

장종산

한국화학연구원 그린화학촉매연구센터

The microwave synthesis method as a green chemical approach has recently attracted growing attention in the synthesis of nanoporous materials that normally require several days for their hydrothermal crystallization. This method has been shown to provide an efficient way to synthesize porous materials with short crystallization times, narrow particle-size distribution, facile morphology control, phase selectivity, and the efficient evaluation of process parameters. In this presentation, we introduce recent work on microwave synthesis, fabrication and applications of inorganic porous materials as well porous metal-organic frameworks (MOFs) as performed by KRICT. Regarding microwave synthesis of metal-incorporated MFI zeolites, it is demonstrated that the coupled effect of metal-incorporation at a suitable concentration level and microwave irradiation during the synthesis of MFI zeolites produces fibrous MFI crystals. We also propose that continuous microwave crystallization system is applicable to large-scale production of porous nickel phosphates and MOFs. Sorption and catalytic properties of porous materials obtained using the microwave method will be also presented as compared with those of the corresponding MOFs prepared by conventional hydrothermal or solvothermal methods.

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발표종류: 심포지엄, 발표일시: 목 17:20, 좌장: 이상기

Green Solvents for Chemicals Synthesis

Tom Welton

Department of Chemistry

The advent of green chemistry has led to the introduction of a number of suggested green solvents. These include supercritical fluids, ionic liquids, highly fluorinated solvents and biomass-derived solvents. In this lecture I discuss the application of these technologies in chemicals synthesis on commercial scales. The successes and failures of different technologies are reported.

대 한 화 학 회
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발표분야: JAIMA Joint Symposium
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Outline of IEC62321 and its revision status

Mr. Koichi Mori

Former Chairman of IEC TC111 (Ex-Fujitsu Limited)

There are many laws and regulations concerning hazardous chemical substances in the world, and harmonized testing measurements of such substances were strongly desired by market. IEC TC111 "Environmental standardization of electrical and electronic products and systems" developed IEC 62321 "Determination of levels of six regulated substances (lead, mercury, cadmium, hexavalent chromium, polybrominated biphenyls, polybrominated diphenyl ethers)" through its WG3. The standard was published in December, 2009 as a horizontal standard. This paper describes outline of IEC TC111 and its WG3 as well as outline of the standard and the background of its standardization work. The paper will also review the results of the WG3 meeting in Kyoto, Japan in April, and refers to a future direction of its revision including issues on additional testing methods and addition of new substances.

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발표분야: JAIMA Joint Symposium
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Persistent Organic Pollutants Accumulated in Crucian carp collected in Japan and Korea

Persistent organic pollutants (POPs) in crucian carp from major river systems in Japan and Korea were determined. The objectives were to compare the concentrations and accumulation profiles of POPs and its candidates in freshwater fish in Japan and Korea and to elucidate the causes of difference between sampling locations and both countries. Biota-sediment accumulation factor (BSAFs) and sex difference in POPs concentration during the spawning season were also studied. POPs surveyed in this study were PCDDs, PCDFs, DL-PCBs, DDTs, drins, chlordane, heptachlor, hexachlorobenzene, mirex and lindane.

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발표종류: 심포지엄, 발표일시: 금 12:10, 좌장: 이석기

Mercury Analysis of Industrial Products by Thermal Decomposition (Gold Amalgamation) Mercury Analyzer

Masashi Taguchi

JAIMA Technical Affairs committee, Nippon Instruments Corporation

EU (European Union) is applying various regulations to poisonous chemicals in industrial products these days. ELV (End of Life Vehicles) Directives(July, 2003), RoHS (Restriction of the Use of Certain Hazardous Substances in Electrical and Electronic Equipment) Directives(July, 2006) including RoHS Directives for Japan and China, and REACH (Registration, Evaluation, Authorization and Restriction of Chemicals) Regulations have been applied to the control of poisonous substances in industrial products. Particularly, mercury is regarded as one of the control targets for specified toxic materials and must be controlled by the industrial manufacturers. Therefore, the measurement of mercury should be done by simple, safe and rapid procedures for multiple samples. The reduction-cold vapor atomic absorption spectrophotometric method which requires the wet pretreatment has been adopted as the official method in many countries. In the meantime, the thermal decomposition (gold amalgamation) method has been discussed as an alternative official analytical method for RoHS –related substances due to the freedom from interfering substances and dangerous reagents and its high sensitivity.In this presentation, the principle, operational easiness and actual measurement examples of the thermal decomposition (gold amalgamation) method and its instrumentation will be explained.

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Analysis of bromine in waste plastics by combustion-ion chromatography

Ryozo Goto

JAIMA Technical affairs committee

The bromine compound used for a plastic flame retardant is a restriction item of RoHS Directive. The bromine compounds of restriction item are PBB and PBDE now. These analyses are difficult the preprocessing, and have various problems. Then, the method of measuring total bromine is simply used. The method of analysis by X-ray fluorescence is used for this measurement. However, this methods of analysis are different the measurement according to matrix and the state of the sample. For this, it is unsuitable for the precise analysis. As for methods of analysis by combustion-ion chromatography, accuracy is good, and the preprocessing is also easy. For this, it is a suitable method for the analysis of total bromine in waste plastics. The outline and the application of this method are described.

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발표분야: JAIMA Joint Symposium

발표종류: 심포지엄, 발표일시: 금 13:30, 좌장: 이석기

Introduction of New Generation Electron Probe Micro Analyzer (EPMA)

Kiyohiro Kohara

Analycal&Measuring Instruments Div., SHIMADZU Corporation

TBA

대한화학회 THE KOREAN CHEMICAL SOCIETY

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장소: 송도컨벤시아

발표코드: **금25B6심**

발표분야: JAIMA Joint Symposium

발표종류: 심포지엄, 발표일시: 금 14:00, 좌장: 이석기

Analysis of Asbestos in bulk Samples

Koyanagi Kazo

Analycal&Measuring Instruments Div., SHIMADZU Corporation

TBA

대 한 화 학 회 THE KOREAN CHEMICAL SOCIETY

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Introduction of JEOL HR/MS for environmental analysis.

Sung-Hee Lee

JEOL Korea Ltd.

Now JEOL Ltd. is supplying various types of Mass Spectrometer for many applications of Mass Spectrometry.Magnetic Sector GC/MS(JMS-800D) and Time-of-Flight GC/MS (JMS-T100GCv) is useful for environmental samples such as Dioxin, Residual pesticides, PCB.Especially high speed screening analysis with TOF GC/MS is good solution for residual pesticides and PCB analysis.Food(Carrot) Extract was used for Residual pesticides sample of this presentation and we could get fast GC/MS measurement data by fast spectrum recording speed.Normally very fast spectrum recording speed is essential for fast GC/MS Measurement and JMS-T100GCv system's recording speed is minimum 0.04 sec(25 Spectra/sec).Almost every measurement is finished in only 6 minutes with this system.

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Asbestos analysis by XRD, and Asbestos regulation

Rigaku Corporation

Application Laboratory, Tomikatsu KUBO(Ph.D)

In recent years, it began to be recognized that asbestos has brought about serious problems in our lives. Many countries governments decided to start to keep asbestos under control. For example, Japanese asbestos regulation became to be much stricter than previous regulation (regulation about content changed from 1.0% to 0.1%). Consequently it is difficult to check the low content asbestos in the construction materials, and high skill technique is required about checking asbestos.In this time, mainly we want to talk about the technique of asbestos analysis by X-ray diffraction method. Normally in the case of analysis of low content asbestos such as 0.1%, it takes long time to make qualitative and quantitative analysis. But if High speed 1D detector can be used, measurement time can be reduced. There are many types of asbestos, and those are complicating structure. It is required that special technique for asbestos analysis in quantitative methods. Therefore we introduce ‘Using high speed 1D detector for asbestos measurement’. ‘About the kind of asbestos’ ‘Asbestos measuring methods in Japan’ ‘Quantitative methods for asbestos analysis’, and we also introduce same example of measurement result about asbestos analysis.

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Utilization of Contemporary LC Technologies

Taketoshi Kanda

Frontier Science Business Division, SHISEIDO CO., LTD

Liquid chromatography (LC) and liquid chromatography/mass spectrometry(LC-MS) are widely used for the analysis of hazardous chemicals. This topic will focus on LC and LC-MS of melamine, the animal drugs, and other hazardous chemicals, using CAPCELL PAK C18, CAPCELL PAK CR and PC HILIC. In addition, one instrumental attempt to reduce carryover in high sensitivity analysis will be mentioned. An autosampler having a new sample introduction mechanism will be discussed.

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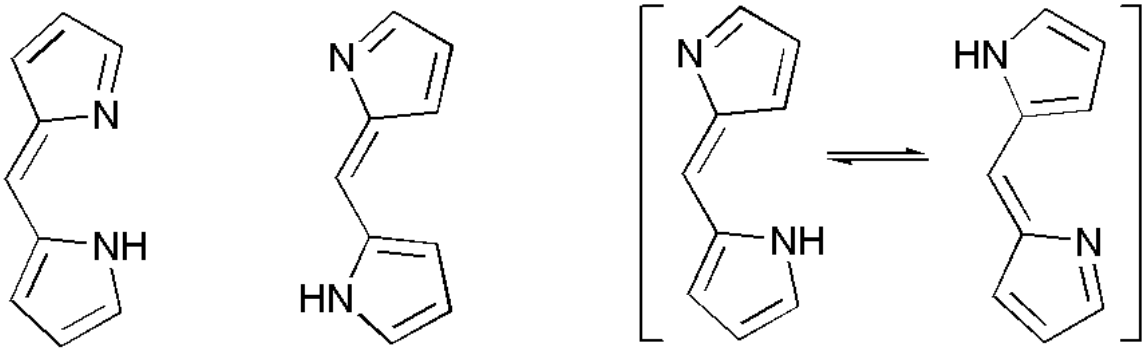
발표분야: 고분자화학 및 재료의 최근연구
발표종류: 구두발표, 발표일시: 금 09:00, 좌장: 최태림

Structural Study of the Self-assemblies Created with Dipyrromethenes

신지영, B. O. Patrick, D. Dolphin, *한재량, 손승배

*Department of Chemistry, University of British Columbia *전북대 화학과*

Study on the alternative dimensional arrangements using diverse flexible-component, the management of intermolecular hydrogen-bonding networks is a powerful tool in crystal engineering. In this presentation, three-dimensional superstructures of the unique self-assemblies generated by exploring the conformational flexibility of various dipyrromethenes through creation of hydrogen-bonds with metal-halide anions are presented and the conformational diversity is thoroughly described in the solid and solution states by X-ray diffraction analysis and variable temperature ^{1}H NMR spectroscopy. Additionally, the molecular arrangements of the self-assemblies formed on graphite surfaces are discussed using scanning tunneling microscopy. The images of the self-assemblies observed on graphite surfaces presented interesting arrangements and appeared as tubular bunches.



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발표분야: 고분자화학 및 재료의 최근연구
발표종류: 구두발표, 발표일시: 금 09:30, 좌장: 최태림

Advanced LCD를 위한 표면 및 계면 처리법

김연상

서울대 나노융합학과

다양한 Display mode 중 LCD(liquid crystal display)는 가장 산업적으로 중심적인 역할을 하고 있다, 특히, 현재 모바일 기기가 주목을 받음에 따라, 이에 따른 다양한 LCD mode 가 새롭게 주목을 받고 있다. 본 발표에서 기존의 LCD 에서의 표면 및 계면 처리의 중요성을 새롭게 소개하고, 차세대 LCD 를 위한 다양한 표면 및 계면 처리법에 대해 발표하고자 한다. 물리적인 구조 및 화학적인 처리가 LC(liquid crystal)의 배향에 어떤 영향을 미칠 수 있는지를 분석하며, 이를 응용한 공정에 대해 최근 경향을 소개하고자 한다.

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Suppressed Dynamics of Polymer Chains in Thin Film Geometry

서영수

세종대 나노공학과

X-ray specula and diffuse scattering were performed on polymer films and analyzed the spectra as a function of film thickness and molecular weight. It has been known that dynamics of polymer chains in thin film geometry are suppressed. For films on the substrate, the effects of the substrates propagate to the surface scaled as a radius of gyration, Rg rather than film thickness and films exactly 2Rg thick exhibit brush-like behavior. For free-standing films, bending modulus of a thin film increases as the film thickness decreases from measuring the integral capillary spectra at the interface between immiscible polymer bilayers. It will be shown that, in both cases, rms roughness on the films exhibits a value as low as few angstrom when the film thickness is less than Rg. Furthermore it will be presented that few angstrom roughness can also be realized for films on engineered surfaces.

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Ion-Permselective Polyelectrolyte Multilayer Membrane modified with pH-sensitive Oxazine Gate

PK JOUSHEED

인천대 화학과

Polyelectrolyte multilayer (PEM) films layer-by-layer deposited on porous supports have been potentially investigated as membrane skins for selective ion separation. The PEM films are known to possess high selectivity of ions due to bipolar nature (Donnan-exclusion effect) with contrast to conventional polymer membrane. The development of stimuli-responsive or switchable membrane is important for technical applications such as filtration system, membrane-based separations, and sensors.This presentation describes a pH-responsive multilayer film composed of two layered components, namely poly(allylamine hydrochloride) (PAH) and a copolymer of acrylic acid and [1,3]oxazine-modified acrylate (POA). The oxazine ring is an acidochromic chromophore, and opens to form either cationic 3H-indolium or anionic hemiaminal in a pH-dependent-manner. This structural transition was used to generate a net positive or negative charge on the membrane for selective ion permeation. The origin of the excellent ion-transport selectivity in the 1 nm ultrathin POA membrane is discussed in terms of alternating charges of the aromatic amphoteric group, oxazine, in the polyeletrolyte membrane.

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발표분야: 고분자화학 및 재료의 최근연구
발표종류: 구두발표, 발표일시: 금 11:00, 좌장: 정병문

Synthesis of Dendronized Polymer by ROMP

최태림

서울대 화학부

Various dendronized polymers (polymers with dendrons attached as side-chain) are synthesized by ring opening metathesis polymerization. (ROMP) These polymers are prepared with not only high molecular weight, but also narrow PDI. Finally dendronized diblock copolymers are prepared via. Atomic force microscopy imaging of individual molecules clearly establishes the presence of structurally distinct blocks.

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Molecular engineering of block and graft copolymers for fuel cell polymer electrolyte membrane

조창기

한양대 응용화공생명공학부

Fuel cell has become one of very hot research topics as one of environmental friendly energy sources. And polymer electrolyte membrane (PEM) is in the heart of the activities for applications as PEM fuel cell or as direct methanol fuel cell. To be a successful PEM material, several requirements have to be satisfied, such as good mechanical and hydrolytic stabilities, low methanol permeability, oxidative stability, good adhesion to electrode, etc. Perfluorosulfonic acid polymer such as Nafion, and many engineering plastics such as polysulfone (PSF) and poly(ether ketone) have been intensively studied because of their outstanding mechanical and hydrolytic stabilities. In this presentation, current research trends and activities of the PEM membranes will be briefly reviewed, and our PEM research activity on the synthesis and characterization of several block and graft copolymers based on PSF and poly(phenylene oxide) (PPO) will be addressed in detail.

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Single Molecule SERS probed by Nano Raman Spectroscopy

서영덕

한국화학연구원 나노바이오융합연구센터 분자고등검지그룹(LAMP)

Since single molecule Surface-Enhanced Raman Scattering(smSERS) was independently reported by S. Nie group and K. Kneipp group in 1997 [1~4], tremendous amount of interest has been shown to this field because Raman spectroscopy can provide molecular fingerprint together with multiplexing capability in bioassay. 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 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 [5].References[1] S. Nie and S. R. Emory, Science. 275, 1102 (1997) [2] K. Kneipp, Y. Wang, H. Kneipp, L. T. Perelman, I. Itzkan, R. R. Dasari, and M. S. Feld, Phys. Rev. Lett. 78, 1667 (1997)[3] A. M. Michaels, M. Nirmal, and L. E. Brus, J. Am. Chem. Soc. 121, 9932 (1999)[4] Y. D. Suh, G. K. Schenter, L. Zhu, and H. P. Lu, Ultramicroscopy 97, 89 (2003)[5] D. Lim, K.-S. Jeon, H.M. Kim, J. –M. Nam, and Y.D. Suh, Nature Materials 9, 60 (2010)

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Quantum Conductance of triple decker sandwich complexes in Au(111) wire-molecule-Au(111) wire

강홍석

전주대 나노신소재공학과

We have calculated the quantum conductance of triple decker sandwich complexes in which Ru and Co ions are sandwiched between five-membered cyclopendadienly groups in Au(111) wire-molecule-Au(111) wire configuration using the Landauer formula. In order to calculate the self-consistent potential under applied bias, the Nonequilibrium Greens's function method is used in combination with density functional theory. Our calculation shows that the systems exhibit nonlinear current-voltage relationshp which is asymmetric with respect to the direction of the applied bias. Multiple negative differential resistances(NDRs) are observed at several applied biases. We find that the underlyling mechanisms are quite diverse: For one of them, the allignment and misallignment of d(Ru) and d(Co) orbitals is a key factor govering the NDR effect, while the coupling and decoupling of surface density of states of Au with the LUMO+1 level of the molecule determines the effect. In addition, an effect of substitution of the hydrogen atom in the central ring by electronegative chlorine atoms on the conductance is also discussed.

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Single-walled carbon nanotube three-dimensional networks: Synthesis and applications for photovoltaic devices

이태재, *서정은, *민선기, *이문근, *여해구, **이하진, *이해원, *한성환

*한양대 나노과학기술연구소 *한양대 화학과 **한국기초과학지원연구원 전주센터*

Carbon nanotubes (CNTs) are an ideal electrode material because of their good conductivity, high aspect ratio with nano-sized diameters, and strong chemical and physical hardnesses. Therefore, CNTs can be used for efficient nano-electrodes in sensors, photo-electronic devices, and alternative sources of energy including solar-cell and fuel-cell applications. Here, we suggest an advanced three-dimensional (3D) electrode structure which consists of high-density single-walled carbon nanotube (SWNT) 3D networks (-3DNs) and a 3D-structured Si pillar template. A Si pillar template was prepared by a deep Si etching process, and the SWNT-3DNs were synthesized over the Si pillars by thermal chemical vapor deposition. Then, a sandwich-type photoelectrochemical (PEC) cell was fabricated by coating the SWNT-3DNs with a quantum dot (QD). SEM, TEM, and Raman analysis was used to characterize the SWNT-3DNs. The results confirmed that the high-density SWNT-3DNs assure the maximum effective density of SWNTs in the confined area of the template. Coating the 3D surface of SWNT-3DNs with functional materials is much important to extend the application fields of SWNT-3DNs. We will also discuss about coating SWNT-3DNs with functional materials by various techniques including an electrochemical deposition and an atomic layer deposition. We expect that the SWNT-3DNs will be useful for fabricating highly efficient nano-electrodes having a large active surface area with the desired spacing.

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Excited-state reversible geminate ABCD reaction in two dimensions

박기현, 신국조, *김효준

*서울대 화학부 *동아대 화학과*

Reversible geminate transfer reaction, A*+B↔C*+D, is studied in two dimensions. For the excited-state transfer reaction with two different lifetimes and quenching, the exact analytical Green functions are generalized for an arbitrary initial condition in the Laplace domain. Long-time asymptotic behaviors of survival probabilities are analyzed in the time domain as well as short-time expressions. The two-dimensional survival probabilities are found to show logarithmic decay behaviors of $(\ln t)^{-1}$ or $t^{-1}(\ln t)^{-2}$ at long times, depending on two lifetimes.

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Fabrication of Surface Plasmon-Coupled Si Nanodots in Au-Peapod-Embedded Amorphous-Silicon-Rich-Oxide Nanowire

권혁상, *박경수, 김성근

*서울대 화학부 *삼성종합기술원 AE 그룹*

Interest in dielctric nanowires containing metal nanoparticle chains continues to grow owing to its potential applications in nanoscale optoelectronics. Simultaneous incorporation of both semiconductor and metal into nanomaterial results in highly desired properties such as local-field-enhanced light emission and improved photoconversion efficiency due to the surface plasmon resonance of metal nanoparticles. Methods of producing silicon oxide nanowires embedded with gold or gold silicide nanoparticle chains have been reported, but in this paper, we report a novel fabrication method for amorphous Si (a-Si) nanodots from gold-nanoparticle-embedded silicon oxide nanowires using irradiation of a low-intensity, parallel electron beam at room temperature. Thermal annealing at 823 K turns a-Si nanodots into and crystalline Si (c-Si) nanodots. Our method produces a high density of Si nanodots with a narrow size distribution, depending strongly on the morphology of gold particles. Characterization of the optical properties of Si nanodots in the vicinity of gold nanoparticles by monochromated electron energy-loss spectroscopy (EELS) reveals a marked enhancement. Furthermore, simple heat treatment at high temperature (1123 K) yields an unexpected Au/Si core-shell nanostructure in the silicon-rich oxide nanowire, with a corresponding plasmon peak redshift.

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Comparative Photophysics on *meso*-alkyl [26]- and [28]Hexaphyrins: Conformational Switching between Hückel and Möbius Aromaticity

윤민철, *Atsuhiro Osuka, 김동호

*연세대 화학과 *Kyoto University, Japan*

Molecular aromaticity in cyclic polyenes has been one of the most important concepts in chemistry over the last several decades. Recently, other types of aromatic compounds have been synthesized based on single-twisted Möbius and double-twisted Hückel aromaticity. In this work, we have investigated on comparative photophysics between *meso*-trifluoromethyl [26]- (TFM26H) and [28]hexaphyrins (TFM28H) to explore aromaticity-correlated photophysics using NMR, steady-state, and time-resolved spectroscopies along with theoretic calculations. It was found that two conformational isomers for TFM28H exist with a fast equilibrium, which is quite sensitive to solvent and temperature. One conformer having short S_1-state lifetime of 10 ps corresponds to the double sided Hückel antiaromatic conformer with figure-eight structure, whereas the other one should have Möbius aromatic nature with 25-fold longer S_1-state lifetime (~250 ps) and highly distorted structure. Through our findings, conformational dynamics on aromatic and antiaromatic mixtures in equilibrium, can provide useful information on the structure-property relationship between aromatic and antiaromatic expanded porphyrin systems.

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Self-Assembly of Nanoparticles into Twisted Ribbons with Light-Controlled Pitch

김상현, 김기섭

충주대 화공생물공학과

Helical structures are among the most ubiquitous in nature due to their unique properties. They are typically produced by the self-assembly of common building blocks of living matter: proteins, amino acids, and oligonucleotides. Like these building blocks, CdTe nanoparticles biomimetically self-assemble into structures that form twisted ribbons. The mechanism of this process is elucidated in detail using both experiments and computer simulation. The pitch of the produced twisted ribbons is controlled by the intensity of illumination in the visible region due to the gradual increase of mechanical stress in the ribbon with greater illumination intensity, which is alleviated by twisting. Beyond biomimicry, the fundamental importance of this study includes: (1) the first demonstration of many-body cooperative processes in a nanoparticle system driven by oxidative evolution of the individual CdTe nanocrystals, and (2) a novel optical effect in nanostructures. This study also demonstrates a viable pathway for the fabrication of nanomaterials possessing helical conformation with fine control of their geometry.

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Prediction of a new amorphous lithium phase at high temperature and high pressure from non-adiabatic electron dynamics simulations

김형준

Center for Materials Simulation & Design, EEWS, KAIST

We recently developed an electron force field (eFF) method for practical non-adiabatic electron dynamics simulations of materials under extreme conditions, and showed that it gave an excellent description of the shock dynamics of hydrogen from molecules to atoms to plasma. Here we apply eFF to the shock dynamics of lithium metal, where we find two distinct consecutive phase changes which manifest themselves as a kink in the shock Hugoniot, previously observed experimentally, but not explained. Analyzing the atomic distribution functions, we establish that the first phase transition corresponds to an fcc-to-cI16 phase transition that was observed previously in isothermal compression experiments, and the second phase transition corresponds to the formation of an amorphous phase of lithium with a novel topology much smaller coordination than in molten lithium and a random connectivity distribution function. This indicates that eFF can elucidate the states of matter under extreme conditions (e.g. warm dense matter).

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Enantioselective [3+2]-Dipolar Cycloaddition of Azomethine Ylide Generated from Nitrone-Alkyne Substrates via Gold Catalysis

정재원, 신승훈

한양대 화학과

8-Azabicyclo[3,2,1]octane forms the common core of wide range of biologically active natural products. Accordingly, efficient synthesis of this skeleton with high level of enantio-control has attracted considerable attention. Recently, our group has been developing nitrone or oxime-mediated redox reactions under the catalysis of Au-complexes. For example, the redox reaction between a nitrone and an alkyne generates azomethine ylide in-situ, in a completely atom-economical fashion which, in turn, participates in a subsequent tandem [3+2] dipolar cycloaddition. However, asymmetric version of this reaction remains unmet challenge yet. Considering the lack of precedents of asymmetric catalysis using Au(III)-complexes, we report here an auxiliary-based approach for the asymmetric [3+2] dipolar cycloaddition. For this purpose, we prepared enantiopure hydroxylamine derivatives and have shown that its nitrone derivatives underwent a smooth Au-catalyzed dipolar cycloaddition with tethered dipolarophiles in >99 % de, and therefore >99 % ee after deprotection of the auxiliary group.

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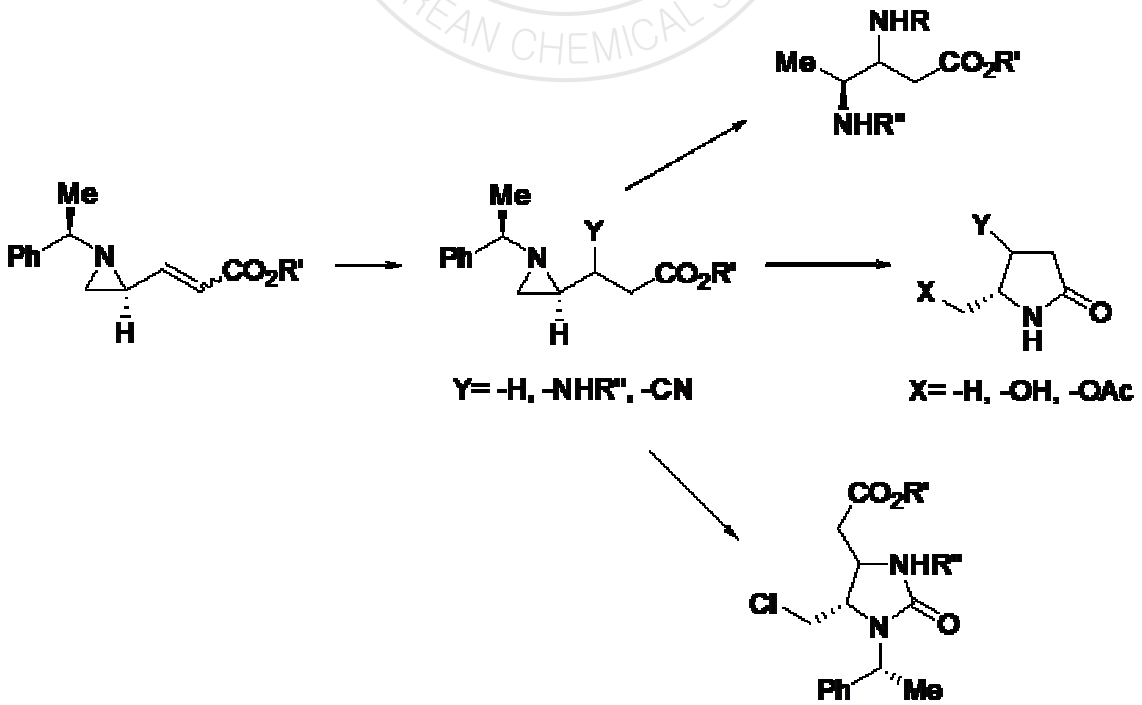
Conjugate Addition of Amine to Chiral 3-Aziridin-2-yl-acrylates.

윤두하, 하현준, *이원구

*한국외국어대 화학과 *서강대 화학과*

Synthesis of stereochemically well-defined 1,2-diamines is still a great challenge to many organic chemists due to their vast utilities as catalysts, metal-ligands and sub-unit of some natural products.Conjugate addition of benzylamine to chiral cis- and trans-methyl 3-[{(1'R)-phenylethylaziridin}-(2R)- and (2S)-yl]-acrylates successfully proceeded to yield 3-aziridin-2-yl-3-benzylaminopropionate in high yield. The additional product was used for the asymmetric synthesis of various 1,2-diamine derivatives including 3,4-diaminopentanoate, 5-chloromethyl-4-alkoxycarbonylmethylimidazolidiin-2-one and 4-amino-5-methylpyrrolidin-2-one.



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Synthesis of Pyrrole Derivatives from Reactions of Propargyl Acetates with Indium Tri(organothiolate)

엄다한, 이필호

강원대 화학과

The sulfide group is a key motif in chemistry and biology. Because of the characteristic features of C-S bond as functions of biological, pharmaceutical, and material sciences, transition metal, such as Pd, Ni, Cu, Co, Rh, and Pt catalyzed C-S bond formations have received much attentions and grown up by means of the development of new catalytic systems and appropriate reagents. Recently, we reported novel and efficient Pd-catalyzed C-C cross-coupling reactions using allylindiums, allenylindiums, tri(organo)indiums, and tetra(organo)indates on the basis of the intriguing chemical properties of indium metal. However, C-S cross-coupling reactions using organoindium reagents have not been reported despite one of the principal methods forming C-heteroatom bonds. These results have led us to investigate the participation of organoindium reagents in C-S cross-coupling reactions. We report that indium tri(organothiolate) are effective nucleophilic coupling partners in Pd-catalyzed C-S cross-coupling reactions with a variety of electrophiles to produce functionalized sulfides and pyrroles in excellent yields.

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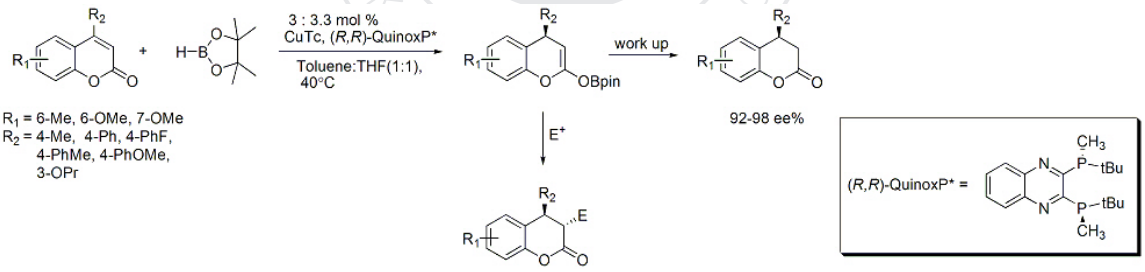
Copper-Catalyzed Asymmetric Conjugate Reductions of Coumarins with Pinacolborane(PinBH)

김효현, 윤재숙

성균관대 화학과

Coumarin derivatives are important in a number of physiologically active compounds. We have developed an efficient enantioselective conjugate reduction of coumarins with copper(I)-QuinoxP* catalyst in the presence of pinacolborane(PinBH) as the stoichiometric reducing agent. We successfully reduced coumarins in high yields with excellent enantioselectivity (up to 98% ee) and developed a catalytic enantioselective aldol reaction with aldehydes or ketones.



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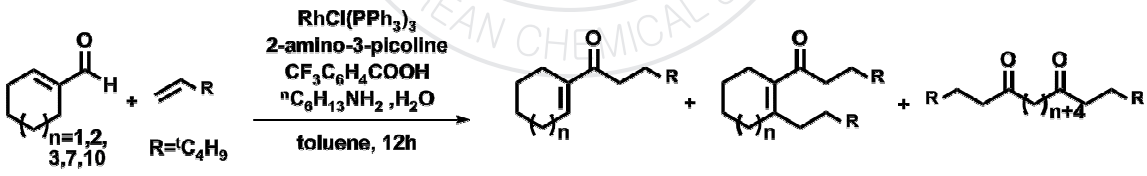
Synthesis of Diketone from Cycloalkene-1-carboxaldehyde through Hydroacylation and retro-Mannich type Reaction

이유라, 전철호

연세대 화학과

Transition-metal catalyzed C-H and C-C bond activation have been widely investigated for the synthesis of useful organic molecules. We have developed novel synthetic method for preparing diketones in one-pot from cycloalkene-1-carbaldehyde and 1-alkene. In this reaction, cycloalkene-1-carbaldehyde was converted to symmetric diketones by consecutive Rh(I)-catalyzed chelation-assisted hydroacylation and amine-mediated retro-mannich type fragmentation. The size of cycloalkene was important for generating diketones. We also applied this protocol to prepare asymmetric diketones using chiral myrtenal.



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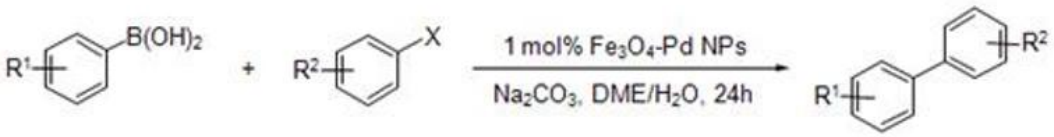
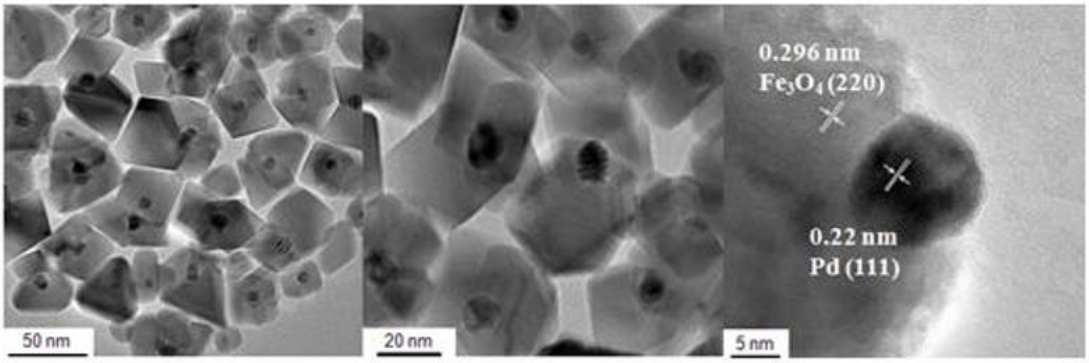
Magnetically Recyclable Palladium Nanoparticles for Suzuki Reactions

정주영

서울대 화학부

Metal nanoparticles show several properties and are regarded as ideal candidates for catalysts. Palladium-catalyzed Suzuki reaction between aryl halides and arylboronic acids has been one of the essential tools for C-C bond formation in organic synthesis. Therefore, reusable palladium nanoparticles that promote these reactions would provide a convenient and practical route for large scale cross-coupling reactions. However, the handling of nanoparticles often imposes problems during work-up. In this regard, we would like to report the use of filtration free, magnetically separable Fe_3O_4-Pd nanoparicle catalysts for the Suzuki reaction. After each reaction, the nanoparticles can be separated from the reaction mixture most conveniently through the use of magnet. Recovered catalysts showed highly conserved reactivity and wide substrate scope under the reaction conditions.





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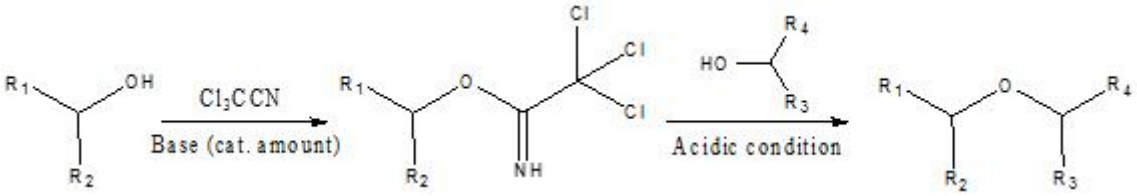
An efficient method for ether formation using trichloroacetimidate

김수정, *박훈규, *김학원

*경희대 화학 및 신소재과학 *경희대 화학과*

Williamson ether synthesis 는 두 개의 alcohol 을 Ether 로 합성하기 위하여 가장 널리 쓰이는 방법이다. 그러나 입체장애가 크거나 basic condition 에 예민한 alcohol 의 경우, 반응시간이 길고, 수득률이 낮아 반응에 어려움이 있다. 이러한 문제점을 개선하기 위하여, acidic condition 에서 trichloroacetimidate 를 사용하여 ether 를 합성하는 효율적인 합성 방법에 대하여 연구하였다. 또한 이를 이용하여 알러지치료제 bepotastin 의 새로운 합성법에 적용하였다.



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Thin-Film Formation of Imidazolium-Based Conjugated Polydiacetylenes and Their Application for Sensing Anionic Surfactants.

김민정, *이경미, **김희진, ***김성진, ****이진용, ***윤주영

*이화여대 화학.나노과학부 *이화여대 바이오.융합대학원 **이화여대 화학나노과학부 ***이화여대 화학과 ****성균관대 화학과*

Polydiacetylenes (PDAs), which can be prepared by the UV irradiation of self-assembled diacetylene (DA) supramolecules, have attracted considerable attention in recent years. The stimulus-induced blue-to-red transition of PDAs has led to the development of a variety of PDA-based chemosensors. we provide the first example of an anionic surfactant-selective sensor based on PDA and imidazolium polymer, which displays fluorescence enhancement and colorimetric changes in the presence of a variety of anionic surfactants. Compared to previous reports, this system is simpler and more effective in sensing anionic surfactants. Remarkably, using the simple colorimetric changes, this system can easily distinguish the two different anionic surfactants, sodium dodecyl sulfate (SDS) and sodium dodecylbenzenesulfonic acid (SDBS), that are used mostwidely in the detergent industry. In conclusion, a new imidazolium-based polydiacetylene was developed as a chemosensor system, which displayed a thin-film structure in a 100% aqueous solution and colorimetric reversibility in the range of 25–50℃. This polymer exhibited selective and unique color changes as well as fluorescence changes when exposed to anionic surfactants. Most importantly, using this system, even SDS and SDBS could be differentiated with the naked eye. To our knowledge, this is the first anionic surfactant sensor based on a PDA. These results are expected to be an important addition to PDA sensor systems.

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Rationally Designed Fluorescence Turn-On Sensors: A New Design Strategy Based on Orbital Control

정효성, *이진용, 김종승

*고려대 화학과 *성균관대 화학과*

We explore a new strategy in the chemo-sensor field for fluorescence amplification upon binding with metal ions based on controlled participation of the nitrogen lone pair orbital. The basic architecture of the sensor entails a fluorophore, the sp^2 hybridized nitrogen lone pair (-C=N-), and a chelator site referred to as the control part. Though nonplanar and nonfluorescent, compound IC1 achieved pseudo planarity from binding with Zn(II) as indicated by the increased fluorescence signal. Its other analogue (IC2), is also planar and not alike IC1-Zn(II), was fluorescent with a lack of binding affinity to metal ions. The time-dependent density functional theory (TDDFT) calculations revealed that the fluorescence amplification was due to the blocking of the nitrogen lone pair orbital; unlikely geometrical rearrangements were insignificant.

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Pyrene Incorporated Calix[4]pyrroles: Synthesis and Molecular Recognition Properties

이창희, 유재덕

강원대 화학과

We have synthesized several new calix[4]pyrroles that bear fluorogenic pyrene as a part of the macrocycle. The synthesized compounds were characterized by proton NMR, HRMS and single crystal X-ray crystalography. The most of the compounds show excellent affinity toward anionic guests as well as some neutral molecules including C70 and polynitroaromatics. Especially, excellent binding affinity was observed to fullerenes with the detection limit of nano-molar range. The emission spectra are dramatically changing depending on the solvent. Monomeric pyrene emission is observed in toluene and pure excimer emission is observed in acetonitrile on the other hand. The detailed binding studies with various guest molecules as well as fluorescence properties will be presented.

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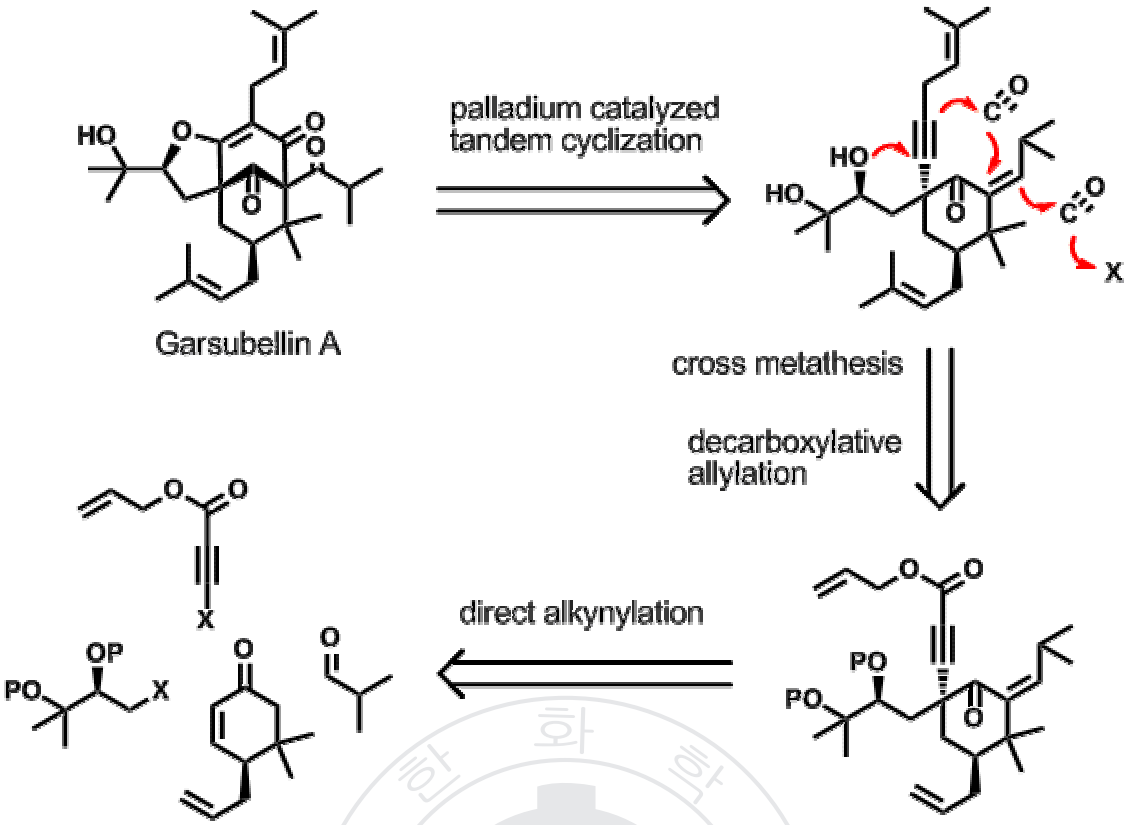
발표분야: 대학원생 구두 발표
발표종류: 구두발표, 발표일시: 금 10:00, 좌장: 신승훈

Synthetic Studies Toward an Enantioselective Total Synthesis of Garsubellin A

장동석

서울대 화학부

Garsubellin A was isolated in 1997 by Fukuyama and co-workers from Garcinia subelliptica which was found on the Okinawa Islands of Japan. Biological investigations revealed garsubellin A to be a potent inducer of choline acetyltransferase (AchT), the enzyme responsible for the biosynthesis of the neurotransmitter acetylcholine. Because the dementia associated with neurodegenerative disorders, such as Alzheimer's disease, has been partially attributed to an atrophy of cholinergic neurons and corresponding deficiencies in Ach levels, garsubellin A could be anticipated to be a promising agent in the treatment of Alzheimer's disease. Presented here is our synthetic studies based upon the proposition that the construction of the tricyclic core of garsubellin A could be realized through a Pd-catalyzed double cyclization of the key precursor containing hydroxyl group, alkyne, alkene functional groups under a CO atmosphere. The details of the results of our studies will be shown in this poster.



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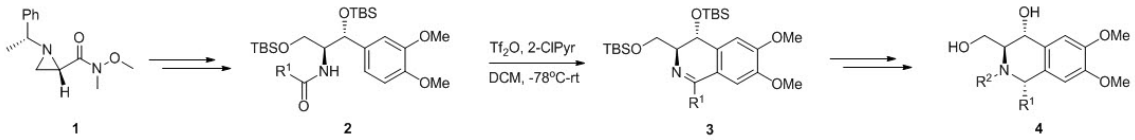
발표종류: 구두발표, 발표일시: 금 10:05, 좌장: 신승훈

Asymmetric Synthesis of 1,2,3,4-tetrahydroisoquinolines from chiral aziridine

김종찬, 강경연, 김준희, 이원구, *하현준

*서강대 화학과 *한국외국어대 화학과*

The Bischler-Napieralski cyclization of chiral (3,4-dimethoxyphenylethyl)amide initiators 2 derived from (S)-N-methoxy-N-methyl-1-[(R)-1-phenylethyl]aziridine-2-carboxamide 1 is an effective method for the synthesis of 3-hydroxymethyltetrahydroisoquinolin-4-ols, which attract interests from chemists due to their biological activities. Stereoselective reduction of the imine product 3 resulted in (1S,3S,4R)-4-(tert-butyldimethylsilyloxy)-3-[(tert-butyldimethylsilyloxy)methyl]-6,7-dimethoxy-1-methyl-1,2,3,4-tetrahydroisoquinolines 4 in high yield.



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발표종류: 구두발표, 발표일시: 금 10:20, 좌장: 전흥배

Total Synthesis of Oxayclic Macrolide Natural Products via Prins Macrocylclization

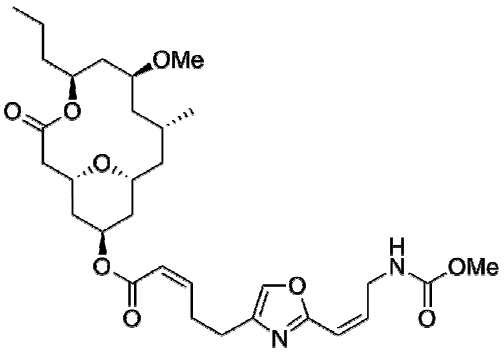
우상국, 이은

서울대 화학부

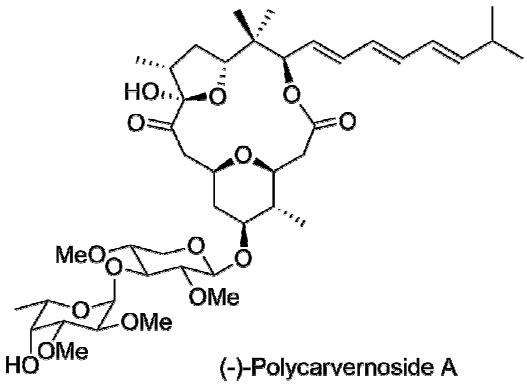
A large number of natural products and medicinally useful agents contain substituted oxacycles. The Prins reaction is one of the methods used for preparation of oxacycles. More recently, intramolecular Prins macrocylclization reaction was successfully employed in the synthesis of oxacylic macrolide natural products.

Neopeltolide is a 12-membered macrolide from a Lithistid sponge of the Neopeltidae family. It is a potent inhibitor of tumor cell proliferation with IC_{50} values of 1.2, 5.1, and 0.56 nM against human lung adenocarcinoma (A549), human ovarian sarcoma (NCI/ADR-RES), and murine leukemia (P388), respectively, and also a potent antifungal agent. Total synthesis of (+)-neopeltolide was accomplished employing intramolecular Prins macrocyclization of an aldehydo homoallylic alcohol intermediate.

Polycavernoside A was isolated by Yasumoto from the edible red alga *Polycavernosa tsudai* as a causative toxin of sudden human intoxication in Guam in 1991. The proposed macrolactone disaccharide structure was confirmed via the first total synthesis of Murai, which also established the absolute stereochemistry. Total synthesis of (−)-polycavernoside A was accomplished employing intramolecular Prins macrocyclization of an aldehydo homoallylic alcohol intermediate.



(+)-Neopeltolide



(-)-Polycarvernoside A

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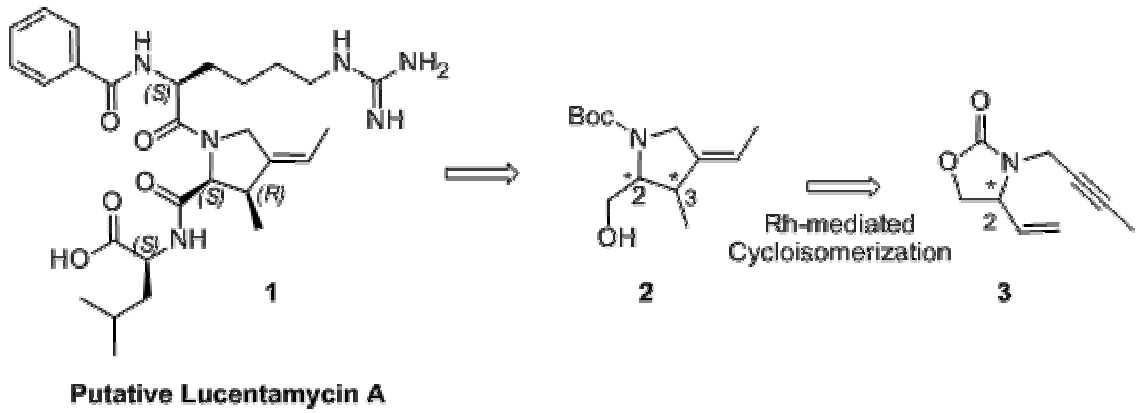
Total Synthesis of Putative Lucentamycin A and Its Analogues by Rh-Catalyzed Diastereoselective Cycloisomerization of 1,6-Enyne

함영진, 최환근, 유하나, *하정미, *심태보

*서강대 화학과 *KIST 생명보건본부*

Lucentamycin A was isolated from Marine-Derived Actinomycete Nocardiopsis lucentensis and showed significant anti-proliferative activity on HCT-116 (colorectal cancer cell) with GI50 value of 0.2 uM. Cho and co-workers proposed a putative structure of Lucentamycin A as illustrated below. In the meanwhile, Juan R. Del Valle group synthesized the putative Lucentamycin A and suggested that the absolute stereochemistry of C-2 and C-3 position of pyrrolidine ring proposed by Cho and co-workers should be revised. By adopting Rh-mediated diastereoselective cycloisomerization of 1,6-enyne system, we successfully developed highly efficient methodology for controlling the configuration of 2,3-substituents on pyrrolidine ring system and applied this to total synthesis of putative Lucentamycin A and its analogues.



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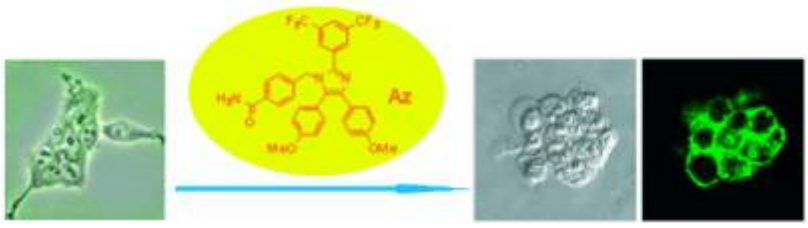
발표종류: 구두발표, 발표일시: 금 11:00, 좌장: 전홍배

A Small Molecule That Induce Apoptosis in Cancer cells

고성균, 김주리, 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. Apoptozole 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.



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Probes for diverse DNA structures using end-stacking, and their applications

이일준, 이정우, 김병현

포항공과대 화학과

Constructing and understanding the functions of biomaterials—DNA, RNA, and proteins—are becoming hot research topics in contemporary science. Especially, monitoring the structural states of the biomolecules in solution phase is important for the understanding of their biological functions. Because noncovalent interactions between aromatic molecules are often important for stabilizing the structures formed from biological molecules, we have synthesized and applied various fluorescent nucleoside derivatives for probing secondary structures of nucleic acid. In oligodeoxynucleotides, not only the stacking between DNA bases but the interaction between the fluorophore and DNA base induce the stable form and make possible of the monitoring the conformational diversity of DNA. By recognizing the interaction between DNA bases and fluorophore, and using quencher-free molecular beacon concept[1], we could design and synthesize various fluorescent oligodeoxynucleotide systems for monitoring various DNA secondary structures, such as B-Z transition[2], G-quadruplex structures[3, 4] and DNA i-motif structure[5]. (1) (a) Hwang, G. T.; Seo, Y. J.; Kim, B. H. J. Am. Chem. Soc. 2004, 126, 6528; (b) Venkatesan, N.; Seo, Y. J.; Kim, B. H. Chem. Soc. Rev. 2008, 37, 648.(2) Seo, Y. J.; Kim, B. H. Chem. Commun. 2006, 150.(3) Seo, Y. J.; Lee, I. J.; Yi, J. W.; Kim, B. H. Chem. Commun. 2007, 2817.(4) Seo, Y. J.; Lee, I. J.; Kim, B. H. Bioorg. Med. Chem. Lett. 2008, 18, 3910.(5) Lee, I. J.; Yi, J. W.; Kim, B. H. Chem. Commun. 2009, 5383.

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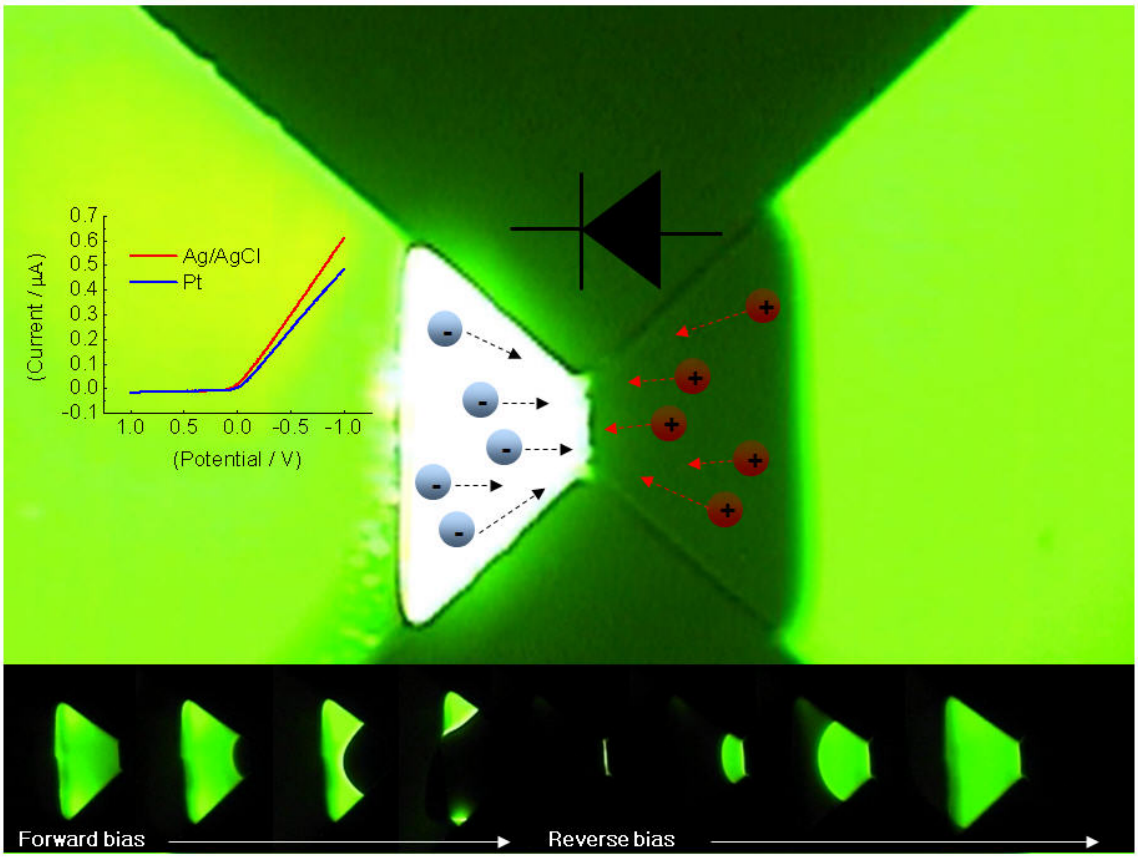
Ionic Circuit based on Polyelectrolyte Diode on a Microchip

한지형, 정택동

서울대 화학부

Polyelectrolyte diode is an electrostatic junction between two oppositely charged polyelectrolytes. This junction system is analogous to silicon-based electronic p-n junction so that it exhibits nonlinear electric behavior like a conventional solid-state diode. Its rectification function upon modulated electric input signals is based on the principle of strong Donnan exclusion. Although the rectified i-v curve due to such a polyelectrolyte system was firstly proposed by Bockris et. al. in 1960, the interpretation of the observed rectified curve was no more than speculation or mathematical simulation. Moreover, there has been only a little advance in the system from his model, which is still far from practical devices. In this respect, microfluidic chip has a great potential to be a platform tool for the intelligent control of ion current as well as real time monitoring, which are expected to inspire many creative devices. Here we report a microchip-based polyelectrolyte diode and a prototype of the integrated system, 'ionic circuit'. The polyelectrolyte diode in this work shows well defined rectification that is purely governed by nonlinear variation of ionic conductance at the micro scale polyelectrolytic junction. In addition, we demonstrate that microchip tool could visualize the dynamic distribution of ions and penetration current by employing fluorescent molecules in real time basis.



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발표분야: 신진 전기화학자 구두발표
발표종류: 구두발표, 발표일시: 금 10:00, 좌장: 이혜진

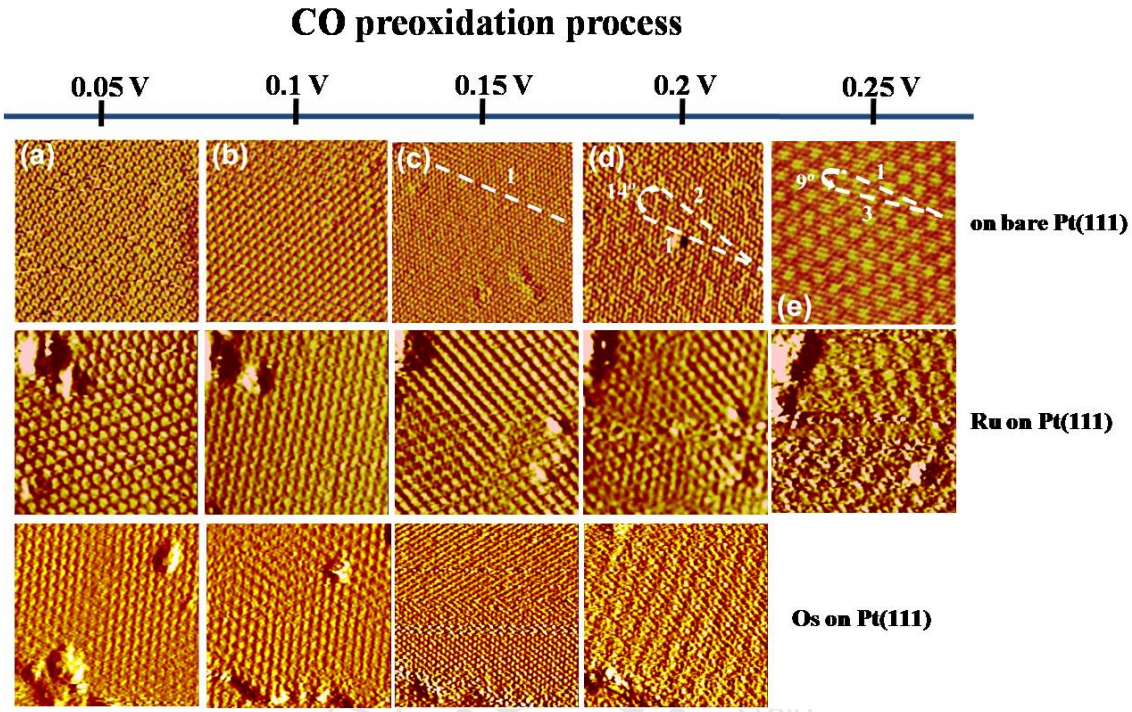
Preoxidation Process of CO on Bare Pt(111), Ru, Os modified Pt(111) Electrode Surfaces

김잔디, 정창훈, 이충균

충남대 화학과

The electrochemical oxidation of CO on Pt surfaces, in particular, has been investigated extensively towards fuel cell technology.[1-4] Various aspects of adsorbed CO molecules and their oxidation have been revealed, because of the relative easiness to access to, with various technique.[4-6]But the details of CO oxidation, e.g. reaction sites, relative rates of charge transfer and surface diffusion of CO, are not yet clearly understood. In 1994, for example, the adlayer of CO on Pt(111) has been reported to transform from a (2×2)-3CO structure to a (√19×√19)R23.4°-13CO structure during the preoxidation (0.0–0.3 V vs. SCE).[7]In this work, presented are sequential electrochemical STM images of CO observed during the preoxidation on bare Pt(111) and Ru, Os-modified Pt(111) electrode surfaces.Sequential images of CO on bare Pt(111) and Ru, Os-modified Pt(111) were observed with electrochemical scanning tunneling microscopy, during its electrochemical preoxidation process. During the preoxidation of CO, the well-known adstructure of CO, (2×2)-3CO-α, was transformed to another well-known structure of (√19×√19)R23.4°-13CO, via (2×2)-3CO-β, (1×1)-CO and (√13×√13)R46.1°-9CO. Such a sequential structural change demonstrates that the structures of (2×2)-3CO-β, (1×1)-CO, (√13×√13)R46.1°-9CO are transient ones during the preoxidation of CO on Pt(111). The presence of Ru and Os on Pt(111) affects the preoxidation in different ways: Ru moves only the main oxidation of CO in the cathodic direction, while Os causes cathodic shifts of the preoxidation and the main oxidation of CO. References[1] Chrzanowski, W.; Wieckowski, A. Interfacial lectrochemistry; Marcel Dekker, Inc: New York, 1999; pp 937-954[2] Iwasita, T. Handbook of Fuel Cells; John Wiley & Sons Ltd.: New York, 2003; Vol. 2, pp 603-624.[3] Maillard, F.; Gloaguen, F.; Hahn, F.; Leger, J.-M. Fuel Cells 2002, 2, 143-152.[4] Yajima, T.; Uchida, H.; Watanabe, M. J. Phys. Chem. B 2004, 108, 2654-2659.[5] Wasberg, M.; Palaikis, L.; Wallen, S.; Kamrath, M.; Wieckowski, A. J. Electroanal. Chem. 1988, 256, 51-63.[6]

Bergelin, M.; Herrero, E.; Feliu, J. M.; Wasberg, M. J. Electroanal. Chem.1999, 467, 74-84.[7] Villegas, I.; Weaver, M. J. J. Chem. Phys. 1994, 101, 1648-1660.



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발표종류: 구두발표, 발표일시: 금 10:30, 좌장: 이혜진

Fabrication and Applications of Potentiometric/Amperometric Conical Glass Nanopore Electrodes

심준호, *남학현, *차근식, **이영미

*이화여대 신재생에너지연구센터 *광운대 화학과 **이화여대 자연과학대학/화학전공*

Truncated cone-shaped glass nanopore electrodes have been fabricated and characterized for their unique electrochemical properties and some potential applications as an electrochemical sensor platform. Herein, we first attempted to use a Pt electrode-based conical nanopore as a transducer of submicro-dimension all-solid-state ion-selective microelectrode (ISME) with reduced membrane resistance and improved analytical performance. The surface of the Pt base in pore is electrochemically coated with silver and then chloridized to obtain intervening Ag/AgCl layer. We investigated the potentiometric characteristics of the fabricated ISMEs, and explored the possibility of using them as probes in scanning electrochemical microscopy (SECM). In addition, we prepared amperometric nitric oxide (NO) microsensors based on a similar Pt electrode-based conical nanopore. The surface of Pt nanopore electrode was electrochemically platinized to enhance the sensitivity. Then the pore glass wall was silanized, and the Pt electrode surface was coated with poly 5-amino-1-naphthol by electropolymerization, which provided the selectivity to NO. Finally, we successfully obtained the images of local NO concentrations for a NO emitting microstructure by employing the NO microsensor as a probe in SECM. This research was carried out under the General R/D Program of the Daegu Gyeongbuk Institute of Science & Technology (DGIST), funded by MEST, ROK.

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장소: 송도컨벤시아
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발표분야: 신진 전기화학자 구두발표
발표종류: 구두발표, 발표일시: 금 11:00, 좌장: 이영미

Synthesis of Hydroquinone Modified Chitosan Derivatives for the Electrocatalytic Sensing of Ascorbic Acid.

Harishchandra D. Jirimali, *신운섭

*서강대 화학과/바이오융합협동과정 *서강대 화학과*

Ascorbic acid (AA) is a water soluble vitamin known for its antioxidant properties and involved in many metabolic activities in human body so it is important to determine the AA. Qinone and hydroquinone compounds participate in the mitochondrial respiratory chain and act as mediator to transport the electrons. Chitosan is a biopolymer obtained by the partial deacetylation of the chitin. In this work hydroquinone modified chitosan derivatives were synthesized by connecting different proportion of hydroquinone moieties to chitosan biopolymer backbone. The modified chitosan hydroquinone polymers were characterized by IR and ^{1}HNMR spectroscopy. Newly synthesized polymer composite with the carbon powder were used for the electrode modification and modified electrode surfaces were studied by SEM. SEM images shows a nano structured composite with uniform coating. Electrochemical properties were studied by cyclic voltametry (CV) and electrochemical impedance measurement. The modified electrodes were utilized for the determination of the ascorbic acid which oxidized at the 0.020 V. Several parameters such as pH and possible interference were investigated with the modified electrode. This nano composite modified electrode shows peak current proportional to the concentration of ascorbic acid in the range of $10x10^{-6}$ to $5x10^{-3}$ M with the detection limit of $5x10^{-6}$ M and sensitivity 0.076 $\mu A \mu M^{-1} cm^{-2}$ for the ascorbic acid sensing.

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발표분야: 신진 전기화학자 구두발표
발표종류: 구두발표, 발표일시: 금 11:30, 좌장: 이영미

Quantum Dot-Sensitized Solar Cells Based on Mesoporous TiO_2 Films

이효중, *박수문

*울산과학기술대 에너지 공학부 *울산과학기술대 에너지공학부*

As for a promising light-harvesting sensitizer, various semiconductors as a form of quantum dots (QDs) and their thin film layers (CdS, PbS, CdSe, CdSe/CdTe, and CdS/CdSe/ZnS) were prepared over mesoporous TiO_2 films by the self-assembling process of pre-prepared colloidal QDs or the successive ionic layer adsorption and reaction (SILAR) process in chemical bath. The as-prepared QD-sensitized electrodes were combined with a redox couple, $Co(o\text{-}phen)^{2+/3+}$ or a polysulfide electrolyte in a liquid type, and then their photovoltaic properties were tested in regenerative sandwich-type cells. Some kinetic parameters were also obtained by using impedance and transient photovoltage decay measurement techniques for the evaluation of those QD-cells. After a series of thorough optimizations in all the components, almost all the tested cells gave over 1 % overall efficiencies and unprecedented high incident photon-current efficiencies (IPCE) when compared to previous results. In particular, multilayered CdSe/CdTe- and CdS/CdSe/ZnS-sensitized cells have showed the best results (3~4 %) among all the cells tested. In this talk, general strategies for making efficient QD- and its dye hybrid-sensitized mesoporous TiO_2 solar cells will be discussed with current limitations and their future prospects of QD-used solar cells.

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발표분야: 화학 교육의 최근 동향과 미래 & 과학 교육과정 프로그램의 현장연구
발표종류: 구두발표, 발표일시: 금 14:00, 좌장: 강훈식

2000년대 화학교육 연구

한재영

충북대 사범대학 화학교육과

2000 년-2009 년 국내외 대표적인 화학교육 및 과학교육 학술지에 게재된 화학교육 관련 연구를 살펴보고 미래 화학교육 연구의 방향을 탐색한다. 국내 학술지로는 대한화학회지와 한국과학교육학회지를 선정하였고, 국외 학술지로는 Journal of Chemical Education 과 Journal of Research in Science Teaching 을 선정하였다. 제목과 초록을 통해 화학교육에 관련된 논문을 선정하고 분류하였다. 논문 내용은 화학 개념 학습과 문제해결, 학습자 특성으로 구분하고, 학교급은 초,중,고등학교, 대학교, 비형식 화학교육 및 교사교육(예비교사, 현직교사, 교수)으로 나누었다. 연구 분야는 반성적 사고, 교육과정 및 평가, 사회-문화-성차, 교육공학, 화학사-철학과 화학사회학, 정책연구 등으로 구분하였다. 연구 방법은 조사연구, 실험연구, 실험연구, 질적연구, 개발연구, 문헌연구 등으로 구분하여 비교하였다. 화학교육 연구를 통해 학문적 발달과 현장 교육 실행의 개선이 동시에 이루어지는 방안을 논의한다.

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발표종류: 구두발표, 발표일시: 금 14:20, 좌장: 강훈식

일본의 새로운 화학 교육과정의 전개

공영태

진주교육대 과학교육과

우리나라의 새로운 과학 교육과정이 개정된 직후인 2008 년 3 월에 일본에서도 초등학교 및 중학교 과학 교육과정에 해당하는 이과학습지도요령(理科學習指導要領)이 개정고시되었다. 이어서 2009 년 3 월에는 새로운 고등학교 과학 교육과정이 개정고시되었다. 이번 교육과정 개정은 1998 년 개정 이래 10 여년만의 전면적인 개정으로, 특히 수학과학 교육이 더욱 강조되어 과학 수업 시간의 증가와 새로운 학습 내용이 신설되는 등 현행 과학 교육과정에 비해 많은 변화를 가져왔다. 또한 내용 영역을 기존의 3 영역에서 2 영역으로 변경하여 제시하고, 내용의 계통화, 국제적 통용성, 새로운 단원의 도입, 표현 활동 등을 강조하고 있다. 일본은 새로운 교육과정의 원활한 적용을 위하여 적응기간인 이행기간을 2~3 년 두고 신 교육과정의 전면적인 실시에 따른 학교현장의 충격을 완화시켜 왔지만 이번인 이행기간 1 년째인 2009 년부터 과학교과는 거의 전면적 실시에 가까운 형태로 새로운 내용의 학습이 도입되는 등 과학교육에 중요성을 두고 있다.

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발표분야: 화학 교육의 최근 동향과 미래 & 과학 교육과정 프로그램의 현장연구
발표종류: 구두발표, 발표일시: 금 14:40, 좌장: 강훈식

수업에 대한 멘토링이 초임 화학 교사의 교수실행에 미치는 영향

The Effect of Mentoring on Beginning Science Teacher's Teaching Practice

박현주, 정대홍

서울대 화학교육과

이 연구는 수업에 대한 멘토링이 초임 화학교사의 교수실행에 어떻게 영향을 미치는지 이해하는데 목적이 있다. 동일한 내용의 수업을 반복하는 과정에서의 멘토링이 교수실행에 직접적인 영향을 미칠 것이라고 판단하여 반복되는 5 차시 수업 상황에서 멘토링이 이루어졌다. 그리고 이것이 멘토링에 의한 교수실행의 변화인지 확인하기 위하여 멘토링없이 진행되는 수업도 5 차시 녹화하여 비교하였다. 연구에는 경력 1 년 미만의 초임 화학교사 2 명이 참여하였고, 각 교사 별로 5 차시씩 2 회, 총 4 주간 수업을 관찰하고, 녹화하였다. 멘토링에는 초임교사를 포함하여 4 명의 화학 교사가 참여하였고, 수업의 장, 단점과 교수실행 개선을 중심으로 논의하였다. 교사의 전반적인 인식을 알아보기 위해 사전 면담이 이루어졌고, 각 차시의 수업 촬영 후 면담이 이루어졌으며, 수업, 멘토링, 면담내용은 모두 전사되었고, 관련 수업 자료, 교사 설문지, 학생 설문지 등을 수집하였다. 연구결과는 다음과 같다. 두 교사의 자발적인 반성에 의한 교수실행은 교수 내용 및 전개 순서, 시간 비중 등에서 약간의 변화가 있었지만, 큰 변화는 관찰되지 않았다. 그러나 수업에 의한 멘토링 이후에는 교사의 과학에 대한 본성, 교수-학습에 대한 가치관 등 교사의 인식 변화뿐 만 아니라, 수업 실행에서의 수업의 목표 선정하기, 다양한 교수학습 전략의 활용, 질문기법을 통한 학생과의 상호작용을 높이기, 효과적인 피드백 제공, 과학 개념의 설명 방식의 변화 등에서 많은 변화가 관찰되었다. 이 연구는 초임 화학교사의 수업 실행에 대한 경험적인 사례 연구로서, 교사의 자발적인 향상보다는 수업에 대한 멘토링이 초임 화학교사의 실제 교수실행에 많은 영향을 미칠 수 있으며, 이를 통해 수업 개선이 이루어질 수 있음을 확인하였다. 또한, 초임교사의 수업 전문성 발달을 위하여 이러한 과정이

필요하며, 보다 체계적이고 구체적인 초임 교사 교육 프로그램 및 연수 과정이 제공되어야 함을 시사한다.

대 한 화 학 회
THE KOREAN CHEMICAL SOCIETY

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발표코드: **금30G4구**
발표분야: 화학 교육의 최근 동향과 미래 & 과학 교육과정 프로그램의 현장연구
발표종류: 구두발표, 발표일시: 금 15:10, 좌장: 강훈식

Interactive Digital Storytelling for Student Motivation

이창재

선문대 화학과

Motivating students to study and learn any subject is not an easy matter. Educators have employed various techniques to engage students' attention. A particularly effective means to attract interest is the use of storytelling. Current generation students respond well to digital media. We took advantage of this trend and have developed a chemistry course in the form of interactive digital storytelling. It is given in the form of a role-playing game, and students have to solve puzzles(chemistry problems) to proceed to the next level (i.e. lecture). The game has been carefully built to avoid cheating, while allowing collaboration. Course log-ins and quiz scores are recorded using PHP scripts and a MySQL database. The semester-end analysis of student attendance and performance reveals that this approach is highly effective in enhancing student motivation and commitment to study and problem-solving skills.

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발표분야: 화학 교육의 최근 동향과 미래 & 과학 교육과정 프로그램의 현장연구
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중등학교 과학(물질) 및 화학교과서에 제시된 실험 안전 관련 연구

박현주, *박윤봉, **현보람

*조선대 과학교육학부 *충남대 화학과 **인천과학고 화학*

실험 수업은 과학의 교수학습 방법을 다른 교과의 교수학습 방법과 구분하는 기준이며, 과학교수의 필수적인 전략이자 그 학습의 수단이다. 실험 수업은 학생들의 인지적인 능력뿐 아니라, 과학적 태도, 과학적 탐구 기능, 과학의 본성 이해, 과학적 개념의 습득 등을 위한 유용한 전략으로 활용되고 있다. 과학교육에서 실험 수업의 중요성과 필요성을 강조하고 있음에도 불구하고, 우리나라 학교 현장에서는 여전히 실험 수업이 잘 이루어지지 않고 있다. 과학 교사의 실험 및 연구에 대한 경험 부족과 시간 부족 등과 더불어, 실험 안전에 대한 불안감은 과학교사들이 실험 수업을 하지 않는 가장 큰 이유 중의 하나로 지적된다. 이 연구는 과학 실험 활동의 안전을 위한 기초 조사로써, 중등학교 과학(물질 분야) 및 고등학교 화학Ⅰ, Ⅱ 교과서의 실험 활동이 내포하고 있는 안전 및 유의사항을 조사□분석하여, 유형별로 구분하였다. 첫째, 과학 실험 활동 안전 및 유의 사항과 관련된 선행 문헌 연구를 통해 실험 활동 안전과 관련된 연구들을 고찰하였다. 둘째, 학년별 1 개 출판사의 교과서를 선택하여 교과서에 제시된 실험 활동을 정리하였다. 셋째, 정리된 실험 활동에서 내포하고 있는 실험 관련 안전 및 유의 사항에 대하여 귀납적으로 조사, 분석하였다. 분석 결과에서 나타나는 실험 안전 사항의 공통 요소를 찾아내어 유형별로 분류하고, 교과서 실험 활동의 안전 사항 분석을 위한 분석틀을 개발, 수정하고 보완하였다. 안전한 과학 실험 활동을 위한 실질적인 정보 제공으로써 과학과 화학 교과서의 실험 활동을 분석한 잠정적 결과, 실험 안전 관련 내용은 교과서에서 실험 활동을 제시하는 방법에서 나타날 수 있는 문제점과 실험 활동에서 실험기구를 통해서나 과정상에 발생할 수 있는 안전 사항 등의 두 부분으로 구분되었다. 그리고 실험 기구나 실험 과정의 안전 사항은 안전 사고와 사례로 세분화되었다.

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초등학교 교사의 탐구자료 활용실태 조사

최취임, *이진승

*서울대 화학교육과 *서울고*

과학교육의 목표는 과학적 소양을 함양시키는 것으로 이를 달성하는데 있어서 탐구가 중심이 되고 있으며, 우리나라의 교육과정에서도 탐구를 강조하고 있다. 탐구중심의 과학교육의 실현을 위해 과학교과서를 탐구중심으로 구성하였으나, 단편적 제시, 개념획득과 이해에 초점을 두고 있으며, 단순탐구 수준으로 구성되어 있어 높은 단계의 사고를 할 기회가 상대적으로 적다. 또한 초등학교는 교사는 탐구를 어떻게 지도할 지에 대한 지식과 경험이 없어 탐구지도에 어려움이 있다. 또한 기존에 개발된 탐구자료들은 즐거움 중심으로 개발되어 학생들의 과학에 대한 긍정적인 태도를 향상시켰으나, 자료들이 대부분 일회성이므로 개념이해 및 탐구기능, 사고력을 단계적으로 향상시키는데 부족함이 있다. 따라서 단편적인 탐구기능학습을 지양하고 실질적인 과학탐구가 이루어질 수 있는 통합적인 탐구활동자료의 개발이 필요하다. 본 연구팀에서는 이러한 문제를 인식하고 구성주의에 기반을 두고 과학개념, 과학탐구기능 사고력학습, 과학적 태도를 함양시킬 수 있는 프로그램을 개발하고자 한다. 본 발표에서는 자료개발에 앞서서 초등학교 교사들의 탐구자료에 대한 요구조사를 실시하고자 한다. 과학교사의 요구조사는 과학교사들이 많이 활용하고 있는 탐구자료 유형, 현재 사용하고 있는 탐구자료에 대한 만족도, 새롭게 개발되는 탐구자료에 대한 요구사항이 무엇인지를 조사하여 발표하고자 한다.

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발표분야: 화학 교육의 최근 동향과 미래 & 과학 교육과정 프로그램의 현장연구
발표종류: 구두발표, 발표일시: 금 16:20, 좌장: 김홍석

STC & STC/MS 프로그램의 소개와 활용가능성 (Introduction to STC & STC/MS curriculum)

이진승

서울고

미래 사회에서는 창의성과 과학적 소양을 갖춘 인재를 요구함에 따라 창의성과 과학적 소양은 과학교육에서 매우 중요하다. 세계의 추세에 맞추어 2007 년, 2009 년 개정 교육과정에서도 창의성과 과학적 소양을 과학의 중요한 목표로 삼고 있다. 이러한 추세를 고려하여 미국과학창의센터가 개발한 과학교육과정의 하나인 STC, STC/MS 프로그램을 소개하고, 이 프로그램과 학습자의 창의성 신장 그리고 과학적 소양 신장의 가능성을 논의한다. 또한, 이를 우리 환경에 맞게 개발한 프로그램도 함께 소개하여 우리 교육 현장에 적용 가능성도 논의한다.

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Cure Properties of New Type Epoxy Resin Systems with Naphthalene Moiety Using 2-methyI imidazole as a Curing Accelerator

전소윤, 김환건, *전현애

*서경대 응용화학과 *한국생산기술연구원 청정소재팀*

Since the requirements of the high density integration and thin packaging technique of the semiconductor have been increasing, the efficiency improvement of the packaging material is quickly advanced. However, there are serious problems due to the moisture absorption and thermal properties of epoxy molding compound (EMC) for semiconductor encapsulation according to the environmental requirements such as Pb free soldering. In this paper, we investigated the cure properties of new naphthalene type epoxy resin(NET-OH, NE-16, NET-Epoxy, NET-MA) systems with 2-methyl imidazole (2MI) as a curing accelerator, which represented high heat resistance and low moisture absorption properties. The cure kinetic parameters of these epoxy resin systems are calculated and reported with dynamic and isothermal approach method using DSC. Among these epoxy resin systems, the lowest value of conversion rate and the highest value of reaction conversion of NET-MA can be observed, which is mainly attributed to the side chain effect of methacrylate group.

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Cure Properties of New Naphthalene Type Epoxy Resin system with Diamino diphenyl methane as a hardener

박숙연, 김환건, *전현애

*서경대 응용화학과 *한국생산기술연구원 청정소재팀*

Because of the growing need for high-density integration and thin-packaging technique of semiconductors, the improvement of packaging materials is progressing fast. In particular, the most significant challenges have been in the area of improving the thermal resistance and moisture resistance of epoxy molding compound (EMC) for semiconductor encapsulation, both to overcome the thermal stress that occurs at reflow soldering and to prevent popcorn crack and warpage of package. In this paper, we investigated the cure properties of new naphthalene type epoxy resin(NET-OH, NE-16, NET-Epoxy, NET-MA) systems with diamino dipheny methane (DDM) as a hardener, which represented high heat resistance and low moisture absorption properties. The cure kinetic parameters of these epoxy resin systems are calculated and reported with dynamic and isothermal approach method using DSC. Among these epoxy resin systems, the highest value of conversion rate and the lowest value of reaction conversion of NET-OH can be observed, which is mainly attributed to the orientation effect of naphthalene group and hydrogen bond of NET-OH.

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Terminally-crosslinked sulfonated poly(fluorenyl ether sulfone) as a highly conductive and stable proton exchange membrane

김태현, roshni

인천대 화학과

The sulfonated poly(fluorenyl ether sulfone) with terminally-crosslinked network structure was prepared by heat-induced crosslinking of the allyl-terminated telechelic sulfone polymers using a bisazide. The crosslinked polymer membrane with a sulfofluorenyl moiety of 70% (PFES-70) showed excellent hydrolytic, dimensional and mechanical stabilities. The conductivity of 0.04 S/cm was obtained for the crosslinked PFES-70 membrane at r.t., and a significant enhancement in conductivity was achieved under heated and hydrated conditions. The conductivity of 0.38 S/cm at 100 °C for PFES-70 was higher than both non-crosslinked (0.33 S/cm) and NafionÒ (0.28 S/cm). In addition, only 2% of methanol permeability (3.9 x 10-8 cm2/sec) compared to Nafion was observed for the crosslinked PFES-70.

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Design And Composition Studies of Electromagnetic Wave Absorbing Rubber-Modified/Epoxy Composite Materials for ISM Band Applications

이준성, 김현규, 김환건

서경대 응용화학과

Many things such as a variety of emerging ISM (the industrial, scientific and medical) equipment and increasing use for wireless device have been become to recognize an important issue needed to protect human body from undesired noise and disoperation of equipment. Since the problem of electromagnetic interference (EMI) of these ISM applications has become serious, much attention has been focused on the electromagnetic wave absorber for reducing the EMI. In this work, we have designed the range of permittivity and permeability of Electromagnetic wave absorber on the basis of contour map method, and investigated the electromagnetic wave absorbing properties of the epoxy/rubber-modified polyamide composite materials with Fe-Al-Si based alloys (sendusts). In order to obtain the high values of complex permittivity and permeability, the shape and content of filler and matrix resin are controlled. The absorption properties of composites decreases with epoxy resin content and the maximum of absorption makes a shift to high frequency, which are attributed to the reflection of electromagnetic wave on the surface of these composites.

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All conjugated block copolymers synthesized via quasi living polymerization

김진석, 박태호

포항공과대 화학공학과

Even though several block copolymers connected with Sp2 carbons, namely, all conjugated block copolymers have been synthesized, exhibiting distinctive optical and electrochemical characteristics it is little attractive partially due to complicated synthetic schemes with low reaction yields and difficulty(or impossibility) in isolating pure block copolymers. Recently, it is successfully demonstrated that quasi living polymerization method using Grignard reagents is a promising method without synthetic difficulty of macromonomers and purification problems to prepare all conjugated block copolymers. We studied reaction mechanism of Grignard reaction at the formation of Sp2-Sp2 carbons connection which involves oxidative addition, metal exchange reaction, and reductive elimination. In addition, we synthesized a class of all conjugated block copolymers applicable to organic electronics, especially, organic photovoltaics. Their phase separation behaviors and organic photovoltaic characteristics will be also presented.

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Separation and determination of hindered-amine light stabilizers by using reverse phase high-performance liquid chromatography/ion-trap mass spectrometry

박인숙, *남궁현

*(주)코오롱 중앙기술원 분석평가연구소 *(주)코오롱 중앙기술원E&A Center*

Quantitative analysis of hindered-amine light stabilizers by using reverse phase high-performance liquid chromatography (HPLC) coupled with electrospray ionization-ion trap mass spectrometry has been performed. A multiple reaction monitoring (MRM) method was used for the detection of various hindered-amine light stabilizers including tinuvin 292, etc. Mass spectrometric parameters were optimized to enhance the detection sensitivity. With this method, very low detection limit of sub-ppm level was achieved with the good linearity (r = 0.999) of the standard calibration curve. The established method was successfully applied to the quantification of light stabilizers in several commercial polymers.

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Preparation and Characterization of Polypyrrole Hybrid Nanoparticles with Controllable Size

Arsalani Nasser, *K. E. Geckeler

*광주과학기술원 신소재공학과 *광주과학기술원 신소재공학과,나노바이오전자재료공학과*

Polypyrrole is an important conducting polymer with outstanding properties. In this study, polypyrrole hybrid nanoparticles were prepared by using an oxidative polymerization process at low temperature in acidic solution and in the presence of poly(ethylenimine) as both the template and amine source. The particle characterization was performed by using FTIR and UV–Vis spectroscopy, X-ray diffraction, thermal gravimetry, scanning electron microscopy, and transmission electron microscopy. It was found that the size of the nanoparticles could be controlled and varied from about 100 to 300 nm with the change in concentration of the reactants. The nanoparticles prepared showed a good dispersability in water with a specific conductivity in the range of 0.1–10 S/cm. Dedoping using sodium hyrdoxide solution changed the optical absorption properties of the nanoparticles but not their size.

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Fabrication of Highly Ordered Silicon Oxide Posts Using Block Copolymer Micellar Templates

유하나, 박수진

울산과학기술대 에너지공학부

We have fabricated highly oriented and ordered arrays of silicon oxide posts via self-assembly of block copolymer containing polystyrene-block-poly(2-vinylpyridine) (PS-b-P2VP) and PS-b-P2VP/PS blend system. Highly ordered PS-b-P2VP and PS-b-P2VP/PS thin films were prepared by solvent annealing in toluene vapor. Then, the nanoporous templates were obtained by the preferential salvation of the P2VP blocks with ethanol. Subsequently, the silicon post arrays were fabricated by spin-coating of PDMS onto the nanoporous templates, thermal annealing, and followed by oxygen plasma treatment. The inter-pore distances can be tuned by controlling the amount of PS added to PS-b-P2VP at a fixed concentration of polymer solution. When a Teflon precursor or polyimide precursor solution was spin-coated onto silicon oxide posts and subsequently dried at certain temperature, flexible nanoporous templates were obtained. This work opens the possibility of use of block copolymer templates for fabricating inorganic nanostructured materials and/or nanoporous flexible nano-reactor.

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Fabrication of Hybrid Donut-like Metal/ZnO Nanostructures by Cooperative Self-Assembly Process

장윤희, 김동하

이화여대 화학나노과학과

Recent studies have focused on unconventional nanostructures based on self-assembly (SA) process that have gained increasing attention due to their unique properties with respect to the traditional low-dimensional analogue nanostructures. Block copolymer self-assembly constitute a typical SA system which enables facile fabrication of functional nanostructures with extraordinary morphology.In this contribution, we suggest a rapid method to synthesize hybrid donut-like metal/ZnO anostructures with ultra-high density and controlled architecture. SA of polystyrene-block-poly(4-vinylpyridine) was combined with sol-gel process to fabricate 2-D arrays of ZnO nanorings. Further, those decorated with Au nanoparticles were also generated by selectively loading Au nanoparticles along the rims of the nanorings. Quasi-hexagonal packed ZnO nanorings with controlled size and dimension were obtained by changing several parameters in mixing protocols. The morphological evolutions of thus obtained hybrid toroidal ZnO nanostructures were monitored by AFM and TEM. We further explore to establish a generalized protocol for the creation of hybrid inorganic-nanoring materials.

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Novel coumarin dyes having EODT moieties for dye-sensitized solar cells: synthesis and characterization

서강득, 주명종, 송해민, 김환규

고려대 신소재화학과

Coumarin dyes with D-low band gap chromophore (ethylenedioxythiophene)-A containing coumarin moiety as the electron donor and cyanoacetic acid moiety as electron acceptor were developed for use in dye-sensitized solar cell. Their chemical structures were characterized by ^{1}H-NMR, FT-IR, UV-vis absorption, and EI-mass spectroscopies. Their electrochemical properties were studied by cyclic voltammetry measurement. These coumarin derivatives have been used to fabricate dye-sensitized solar cells based on I^-/I_2 liquid electrolytes as dye sensitizers and their device performances were evaluated by comparing with that of Ru dye and NKX-2677 dye.

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Synthesis of graphene nanosheet/polyaniline composite in basic medium and its propreties

김진화, 김기연, 오웅주

명지대 화학과

Recently the synthesis of graphene - polymer composite to improve the processibility of graphene has been reported. In the case of graphene nanosheet-polyaniline composite was synthesized in acidic medium (pH ~2) but poor dispersion stability was a problem to be solved. In this study graphene nanosheet-polyaniline composite was synthesized in basic medium (pH 9 ~ 11) based on Donnan effect. SEM and XRD was used to investigate the structure of the composite. Electrical conductivity and tensile strength was measured from free standing film made with the dispersion. Zeta potential was monitored to check the stability of the dispersion. Effect of pH value to the properties of graphene nanosheet-polyaniline composite will be discussed.

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Thermal and weathering degradation of poly(propylene carbonate)

KodiyanVarghese Jobi

아주대 분자과학기술학과

High molecular-weight poly(propylene carbonate) (PPC) is intact when it is stored in an ambient air or in a water for 8 months once the catalyst is completely removed. The catalyst-free pure PPC is also thermally stable below 180°C. At 200°C, substantial alteration is observed on the GPC curve. Main degradation mechanism of the pure PPC is an attack of the chain-ended hydroxyl group onto a carbonate linkage, through which the molecular weight distribution is broadened by simultaneous formation of low and high molecular weight fractions. Incomplete removal of hydrogen peroxide, generated during the catalyst preparation results in a prepared polymer contains a substantial amount of polymer chains grown biaxially from the hydrogen peroxide, which resulted in more severe thermal degradation. Experiments conducted in weathering chamber at high temperature (630°C) and high humidity (50%) revealed another degradation process involving chain scission through an attack of water molecule onto the carbonate linkage - additionally operates, which progressively and temporally lowers molecular weight.

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Synthesis and Properties of Novel Low Bandgap Polymer Based on Cyclopentadithiophene

박세정, 신현민, 서홍석

부산대 화학과

Many conjugated polymers for solar cells were synthesized. P3HT and PCPDTBT were successful OPVs. New type for OPVs is D-A polymers which have two absorption band in UV-vis absorption spectra. These UV absorption bands can cover large area of solar spectrum. Recently, derivatives of PCPDTBT were synthesized and reported high photovoltaic properties. We designed and synthesized new acceptor material for D-A polymers. Novel conjugated polymer PCPDTMBI based on CPDT(cyclopentadithiophene) was synthesized by Stile coupling. The number molecular weight (Mn) of PCPDTMBI was 8.5 kg/mol, and the polydispersity index (PDI) was 2.1. UV-vis spectra of PCPDTMBI showed two band. Two λmax were 430 nm and 730 nm. Eopt was about 1.30 eV.

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Low-Bandgap PCPP Derivatives Introduced 4,7-Dithienyl-2,1,3-benzothiadiazole Unit for Photovoltaic Cells

박세정, 한효정, 서홍석

부산대 화학과

Novel conjugated polymer bearing 4H-cyclopenta[def]phenanthrene (CPP) unit have been synthesized and was evaluated in bulk heterojunction solar cell. The alternating copolymers with CPP unit were synthesized with 4,7-dithienyl-2,1,3-benzothiadiazole (DTBT) unit by Suzuki coupling polymerization. The newly synthesized copolymers, poly(2,6-((4,4-bis(2-ethylhexyl)-4H-cyclopenta[def]phenanthrene))-alt-(4,7-((2-thienyl)-2,1,3-benzothiadiazole))) (PCPP-DTBT), and poly(2,6-(4,4-bis(4-((2-ethylhexyl)oxy)phenyl)-4H-cyclopenta[def]phenanthrene)-alt-(4,7-((2-thienyl)-2,1,3-benzothiadiazole))) (PBEHPCPP-DTBT), contain dialkyl and bis(alkoxyphenyl) groups in the CPP unit, respectively. Both of conjugated polymers showed significant absorbance up to around 700 nm region. The HOMO-LUMO energy bandgaps of these materials, estimated from UV-vis spectroscopy and cyclic voltammetry (CV), were 2.00 eV for PCPP-DTBT and 1.80 eV for PBEHPCPP-DTBT. Bulk heterojunction solar cells based on the blends of the polymers with [6,6]phenyl-C71-butyric acid methyl ester (PC71BM) gave power conversion efficiencies as 1.00% for PCPP-DTBT and 1.12% for PBEHPCPP-DTBT under AM 1.5, 100 mW/cm2.

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Mussel-inspired catechol PEG hydrogels

홍선기, 이해신

KAIST 화학과

Poly(ethylene glycol) (PEG) have been exhaustively used for biocompatible hydrogels. Herein, we developed a new biomimetic approach for the formation of PEG hydrogels. Catechol, an enediol-containing small molecule, inspired by the adhesive amino acid 3,4-dihydroxy-L-phenylalenine (DOPA) was end-functionalized to 6-Arm PEGs (Mw 15,000) (6PEG-catechol). In particular, two different catechol end-functionalization approaches were used; amide and amine were formed as a result of the end-functionalization (6PEG-amide-catechol and 6PEG-NH-catechol). All hydrogels showed successful gelation with strong mechanical properties. However, the two 6PEG-catechols exhibited difference in gelation time and/or mechanical properties. Our result indicates that linker chemistry could significantly influence resulting properties of PEG hydrogels.

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Hydroxy Substituted 2-Phenyl-naphthalenes as a New Candidate for Depigmentation Reagents

송수희, 한효정, 손인영, 서홍석

부산대 화학과

Our present study demonstrated that HPN inhibited tyrosinase and that HPN were able to reduce melanin content without showing any adverse effect on cell viability. We suggest that HPN's melanogenesis inhibitory property acts through the inhibition of tyrosinase. The inhibitory action of HPN (IC50=15.2 μM) on mushroom tyrosinase was revealed. To further explore the action of HPN on melanogenesis, the inhibition of tyrosinase and melanin levels were measured in B16 melanoma cells (B16cells). We examined the inhibitory action of HPN on the tyrosinase activity, and data shows that HPN had a strong suppressive action on the enzyme, at the IC50 value of 1.52×10-5 M. When compared with resveratrol (IC50=5.68×10-5 M), HPN was shown to have more powerful effect than resveratrol. Based on these findings, we suggest that HPN could potentially be a useful skin-lightening agent.

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Synthesis and Properties of Novel Conjugated Polymer Introduced Dimethyl-Benzimidazole Moiety for OPVs.

송수희, 한효정, 심주영, 서홍석

부산대 화학과

New conjugated polymers containing electron donor-acceptor pairs for organic photovoltaic device utilizing a new type of acceptor, dimethyl-2H-benzimidazole, are reported to show good solubility at room temperature in organic solvents. These donor-acceptor conjugated polymers were synthesized by Suzuki coupling reaction of 2,2-dimethyl-4,7-di(2-thienyl)-2H-benzimidazole and donors including carbazole, 4H-cyclopenta[def]phenanthrene and fluorene. The new type of acceptor was fabricated in PCDTMBI, PCPPDTMBI and PFDTMBI.

한국화학회 KOREAN CHEMICAL SOCIETY

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Novel Conjugated Polymers of Polyfluorene Derivatives and C60

진영읍, *송수희, *신현민, *박세정, *서홍석

*부경대 공업화학과 *부산대 화학과*

New polyfluorene (PF)-based conjugated polymers, PC60BEHF, PC60BEHF-co-PDEHF containing chloro, azido, piperidine, and fullerene (C60) groups as pendants, were synthesized. The bulk heterojunction devices were fabricated with a typical device structure of ITO/PEDOT:PSS/composite film/Al. Solar cell was characterized under 100 mW/cm2 white illumination from Halogen lamp (LS-F100HS Light Bank). The band gap of polyfluorene is higher than MEH-PPV, and also acts as the barrier for the charge transfer between MEH-PPV to C60. As a result, the performance of the device using PC60BEHF-co-PDEHF, which has more amount of polyfluorene, showed the lower Jsc, Voc and FF as compared to those of the device using PC60BEHF. we can conclude that alkylated polyfluorene derivatives with C60 have a defect in electron transfer to electrode and too high bandgap for solar cells.

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Synthesis and Properties of Novel Polyfluorenevinylene with Cyano Group and Carbazole Unit

송수희, *진영읍, 손인영, 심주영, 서홍석

*부산대 화학과 *부경대 공업화학과*

To generate red shifted emission as compared to PFs, vinylene unit has been introduced in PF to generate poly(fluorenevinylene)s (PFVs). The present investigation deals with the synthesis, characterization and EL of new copolymers, CzCNPFVs CzCNPFV1, CzCNPFV2 and CzCNPFV3 to improve the device performance as compare to that of PFVs. The new copolymers were synthesized by by the Knoevenagel condensation, the carbazole pendant was introduced to improve the efficiency of reported CNPFV. The PL emission spectra of the CzCNPFVs in chloroform solution show maximum peaks at 476 ~ 479 nm. In thin films, maximum peaks of the CzCNPFVs appeared at 501 ~ 504 nm, red-shifted around 25 nm as compared to those in solution. The emission maxima of the EL spectra of the polymers appear at around 496 ~ 504 nm. The maximum luminescence (Lmax) of CzCNPFV2 of the device with the configuration of ITO/PEDOT/CzCNPFVs/Ca/Al is 1724 cd/m2 at 8 V. The maximum luminescence efficiency of CzCNPFV1 is 0.18 cd/A.

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Synthesis and Properties of Novel Resveratrol Analogue Substituted 2-Phenylnaphthalenes Treatment

송수희, 손인영, 한효정, 서홍석

부산대 화학과

Oxyresveratrol and resveratrol, with hydroxy substituted trans-stilbene structure, exert potent inhibitory effects on cyclooxygenase, rat liver mitochondrial ATPase activity, and tyrosinase. Bcl-2 protects cancer cells from the apoptotic effects of various chemotherapeutic agents. Inhibition or down regulation of Bcl-2 represents a new therapeutic approach to bypass chemoresistance in cancer cells. Previously we designed and synthesized the resveratrol analogue HS compound displaying stronger antitumor efficacy than resveratrol and further demonstrated the HS compound resistance conferred by Bcl-2 in human leukemic U937 cells. Various apoptosis assessment assays demonstrated that HS compound overcomes the resistance conferred by Bcl-2 in Caki-1 cells by inducing apoptosis.

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BBr3-promoted cyclization to ladder-type CPs; synthesis , properties and application

이명건, 김태현

인천대 화학과

Novel chemical cyclization methods using BBr3 have been successfully developed to produce ladder-type conjugated molecules. Having the planar structure and extended pi-conjugation, together with rigid laddery structure, we expect an interesting optoelectronic behaviour for these newly-made CPs. Both electron-rich and poor materials can be easily obtained, hence their application to OFET is under investigation. Synthesis of the novel ladder-type CPs, their physical and electrical properties will be detailed.

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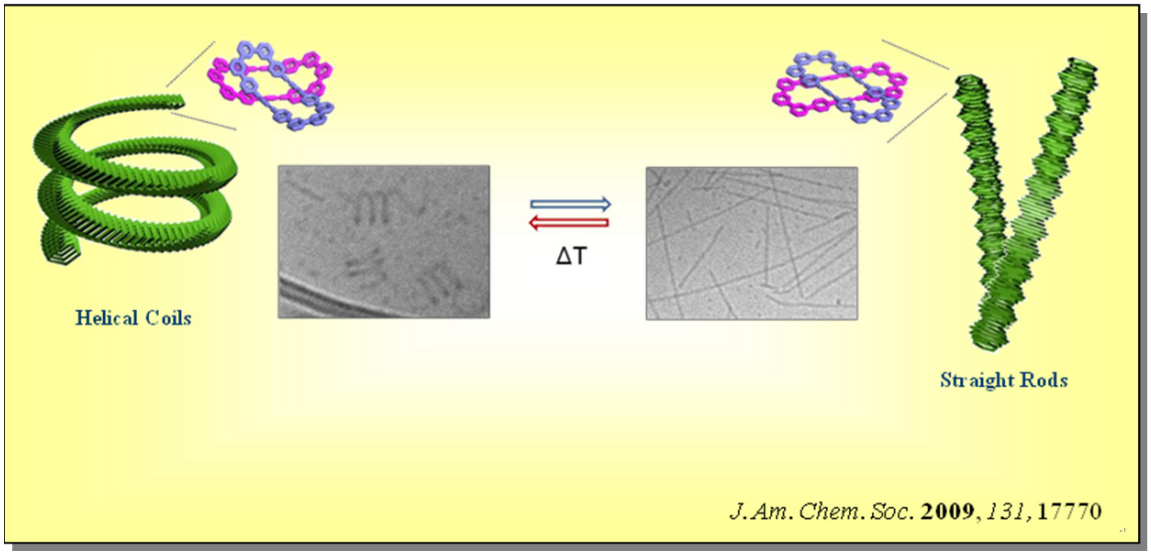
Reversible Transformation of Helical Coils and Straight Rods in Cylindrical Assembly of Elliptical Macrocycles

김태훈, 이명수

서울대 화학부

We have synthesized amphiphilic aromatic macrocycles with an elliptical shape containing oligoether dendrons that can endow aggregates with a thermoresponsive feature. The most notable feature of the elliptical macrocycles investigated here is their ability to self-assemble into helical coils. The helical coils, a significant contrast to others, reversibly transform into straight rods upon heating while maintaining the supramolecular chirality. This structural transition is accompanied by conformational change of the elliptical macrocycles from a boat conformation to a more planar conformation. Such cylindrical aggregates with dynamic structural changes may provide a new strategy for creating intelligent nanomaterals with internal channels.



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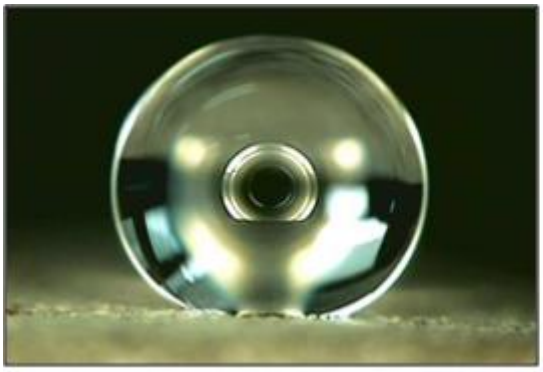
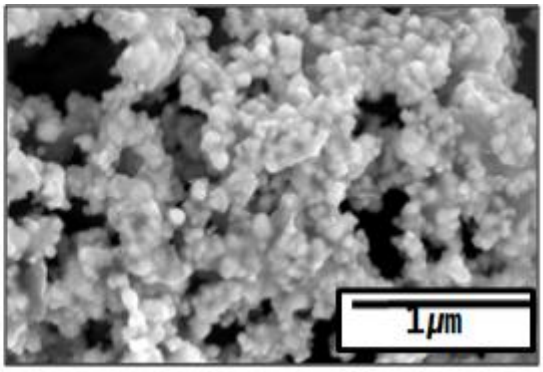
Preparation of Super-Hydrophobic Surface on Magnesium Surface

박연화, 안용현

단국대 화학과

The wettability of solid surfaces is of great interest in daily life and industry. Wettability is controlled by both the geometrical structure of a surface and alow surface energy material coating. A superhydrophobic surface is satisfied with a water contact angle of more than 150° and a sliding angle of less than 10°. The wettability of solid surface is controlled by both the chemical compositions and geometrical nano structure of the surface. In nature, this is the lotus effect. We synthesized silane derivatives and developed the method to fabricate a super-hydrophobic surface by the silane derivatives. We used the process of chemical deposition to deposit metal clusters on a magnesium plate and then simply modified the plate with silane derivatives. The hydrophobic surfaces were obtained by dip-coating the solutions prepared via hydrolysis and condensation of silane derivatives onto metal surface. The morphology of coated surface was characterized by SEM





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Study of poly(norbornene biimides)s with various side groups

윤경환, 윤도영

서울대 화학부

Poly(norbornene biimides)s with various side groups were synthesized by ring opening metathesis polymerization using Grubbs catalysts. Structural characterization was done by GPC, NMR, IR and WAXD. Their physical, optical and dielectric properties were studied for potential application in electronic devices.

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Tubular Stacking of Water-Soluble Toroids via Fullerene Encapsulation

강성균, *이명수

*서울대 화학부 *서울대 화학과*

Construction of one-dimensional (1D) tubular structures by self-assembly of designed molecules has attracted considerable attention because of their potential applications and practical implications. Recently, we have prepared water-soluble toroids with a hydrophobic interior through the coassembly of laterally grafted amphiphilic molecules. We verified internal cavity in the barrel-like toroids, then we introduced fullerene(C_{60}) as a guest molecule. After addition of C_{60} to the solution, the fluorescence intensity was significantly quenched, indicating that C_{60} was effectively encapsulated within the hydrophobic interior of the rings. Encapsulation of C_{60} forces the toroids to pile up on the top of each other and it finally forms a tubular container.

J. Am. Chem. Soc. 2009, *131*, 18242-18243

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Direct sulfonation of polystyrene-b-polybutadiene-b-polystyrene (SBS) for application to proton exchange membrane (PEM) for DMFC

김슬기, 이원목

세종대 화학과

Recently researches have been conducted about development of proton exchange membrane(PEM) for direct methanol fuel cell (DMFC). In this study, sulfonated polystyrene-block-polybutadiene-block-polystyrene(SBS) PEM for the application of the membrane electrode assembly(MEA) was synthesized and investigated. PS and PB blocks were partially sulfonated using acetyl sulfate, and microphase-separated SBS exhibited high ion conductivity. Degree of sulfonation was analyzed by IR, DSC and EA. Double bonds in PB chains were cross-linked by photo-initiator to enhance a mechanical property of the membrane. Ion conductivity, MeOH permeability and water uptake of sSBS PEMs depending on degree of sulfonation were measured and compared to those of Nafion. Cross-linked sSBS membranes showed better mechanical, thermal properties and oxidative stabilities compared to non cross-linked sSBS membranes. Sulfonated SBS membrane was fabricated into MEA, and in active mode DMFC test for these MEAs showed similar performance to that made up of Nafion.

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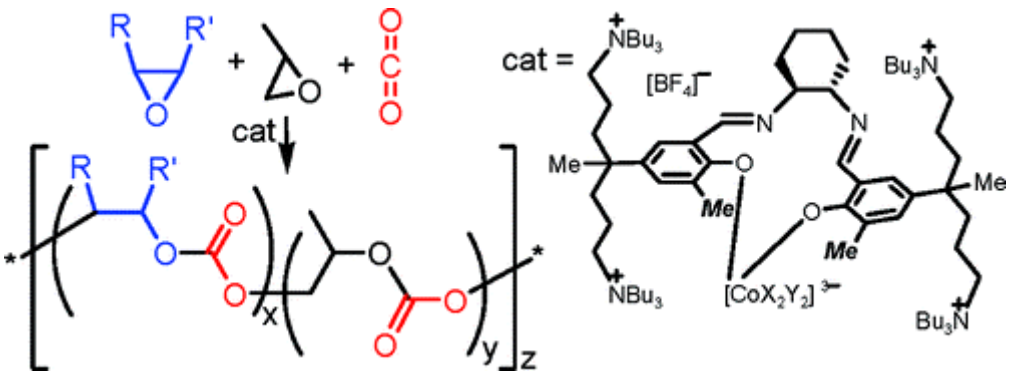
Terpolymerizations of CO_2, Propylene Oxide, and Various Epoxides Using a Cobalt(III) Complex of Salen-Type Ligand Tethered by Four Quaternary Ammonium Salts

이상환

아주대 분자과학기술학과

Terpolymerizations of CO_2/propylene oxide (PO)/cyclohexene oxide (CHO), CO_2/PO/1-hexene oxide (HO), and CO2/PO/1-butene oxide (BO) were carried out without the formation of cyclic carbonates and ether linkages with a cobalt(III) complex of a Salen-type ligand tethered by four quaternary ammonium salts. The activities were excellent, in the range of (0.62-1.6) x 10^6 g/mol-Co (TOF, 4400-14 000 h^{-1}). In all three of terpolymerizations, the data for the PO mole fractions in the feed (f_{PO}) and the polymers (F_{PO}) fit the Fineman-Ross plot well to determine the monomer reactivity ratios. Thelinear dependencies of the T_g's of the polymers on the mole fractions of the third monomers (F_{CHO}, F_{HO}, and F_{BO}) were observed with the relationships of "T_g (°C)=81 x F_{CHO} + 40", "T_g (°C)=-62 x F_{HO} + 38", and "T_g (°C)=-27 x F_{BO} + 38", respectively. The decomposition temperature of the resin increased when the third monomer was employed. The GPC data indicated that the polymer chains grew in an immortal passion from four 2,4-dinitrophenolates as well as the two 2,4-dinitrophenols catalyst bears. High molecular weights (M_n) above 200,000 were attainable because of the high activities.



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Fast Responsive Dual Tunable Photonic Crystal Sensor Based on Templated Photo-Polymerization of Hydrogel Inverse opal

신진섭, *한민수, 이원목

*세종대 화학과 *중앙대 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. Sensing 원리는 pH 나 온도, chemical molecules 등의 외부자극에 의해 주기적인 구조의 체적이 변하여 회절광의 색이 바뀌기 때문에 센서로서의 작용이 가능하다. 하이드로젤 센서는 전구물질인 2-hydroxyethyl methacrylate (HEMA)와 공중합이 가능한 vinyl 기를 가지고, 가역적인 binding 을 할 수 있는 sensing monomer 만 있다면 원하는 검출물질을 쉽게 sensing 할 수 있다. 본 연구에서는 polystyrene 구형입자로 자기 조립 콜로이드 결정을 제작하고, HEMA 와 다양한 sensing moiety 를 광개시제와 콜로이드 결정에 주입하여 최적화된 방법으로 hydrogel inverse opal 을 제작, 다양한 analyte 를 sensing 하였다. 연구결과 pH, 온도, 전이금속 이온, 카이랄 분자 등의 자극에 대해 가시광선 영역에서 대면적의 빠른 색 변화를 육안으로 관찰하였다. 그리고 HEMA 와 온도감응 물질인 N-isopropylacrylamide (NIPAm)을 공중합하여 pH 와 온도에 대한 감응을 동시에 관찰할 수 있었다.

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Thermally crosslinked polysulfone membranes for Direct Methanol Fuel Cells (DMFC)

길승철, *김슬기, 이원목

*세종대 화학과 *세종대 응용화학과*

DMFC 는 메탄올을 직접 연료로 사용하여 장치가 간단하며, 연료 저장의 효율성 등으로 이동용 공급 전원으로서 큰 관심을 받고 있다. Polysulfone 은 높은 유리전이 온도를 가지고 있으며, 열적, 기계적 안정성이 우수하므로 Nafion 대체 PEM 으로 가능성이 높다. 본 연구에서는 Polysulfone 을 DMFC PEM 에 적용하기 위해 단량체 DCDPS 를 설폰화하였고. 설폰화된 DCDPS, Bisphenol A, DCDPS 의 축합중합반응을 통해 설폰화도를 조절하여, phase transfer reaction 을 통해 가교 가능한 반응성 말단기(allyl 기, propargyl 기)를 도입하였다. 합성된 polymer 를 열가교하여 In-situ crosslinked membrane 을 제조하였으며, 그 물성을 측정, 비교하였다.

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Excimer Emission from Nanostructured Pyrene Block Copolymers Prepared by Atom Transfer Radical Polymerization

유정목, *Jeong-Ae Yoon, 김정훈, *Chih-Feng Huang, *Krzysztof Matyjaszewski, 김은경

*연세대 화학공학과 *Department of Chemistry, Carnegie Mellon University, USA*

Well controlled fluorescent block and random copolymers were synthesized by atom transfer radical polymerization (ATRP) of methyl methacrylate and 1-pyreneylmethyl methacrylate, respectively. The fluorescence spectra of the random copolymer exhibited both monomer and excimer emission of pyrenyl units, while the block copolymer exhibited a strong excimer emission with a negligible monomer emission because of the closely bound pyreneyl units on the polymer backbones. Self organization and phase transition of pyrene containing block copolymers could be further controlled by heat. The effect of nanoscale confinement of the polymers above glass transition temperature on their fluorescence properties was investigated by a spectroscopic method in combination with TEM studies. Dramatic changes of the fluorescence intensity and the emission wavelength were observed and they could be attributed to the rearrangement of the fluorescent blocks through a thermally induced self assembly.

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Organic Photovoaltaic Based on Conjugated Polymer using Indenoindene and Benzimidazole

심주영, 송수희, 서홍석

부산대 화학과

Low band gap conjugated polymers with proper energy levels for charge transfer are required to achieve high-efficiency polymer solar cells. We have synthesized new conjugated polymers using indenoindene and benzimidazole with dithiophene as the building block. Since the copolymers including indenoindene and benzimidazole units have stable backbone, high solubility and low band gap, they can be utilized as efficient electron-donating materials for the photovoltaic devices. The best solar cell performance obtained has a layered structure of ITO / PEDOT:PSS / PININEDTMBI:PC71BM(1:4) / Al. Under white light illumination (AM 1.5 G, 100 mW/cm2), the obtained Jsc is 2.38 mA/cm2, Voc is 0.82 V, FF is 38%, and PCE is 0.76%. All of the results were calibrated by the spectral mismatch of our measuring system. Study to improve the solar cell architecture and PCE is underway.

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Defect Elimination and Improved Catalytic Efficiency of ZnO Nanowire Decorated with Gold or Silver Nanoparticles

Saji Thomas, 김동하

이화여대 화학나노과학과

In recent years, researches on one-dimensional (1D) nanostructured semiconducting materials have been stretched to a wide extent, due to their potential applications in mesoscopic physics and nanodevices. Zinc oxide (ZnO) nanowires (NWs) are promising semiconducting material due to their large surface-to-volume ratio and the photon confinement effect. Doping of ZnO with noble metals can be used as effective method to reduce the defect loss, since the visible emission of ZnO remains as a major obstacle for the fabrication of high-efficiency solid state emitters. Here, we use block copolymer (BCP) as a template to fabricate strings of ZnO nanoparticles (NPs), arranged in NW fashion. Polystyrene-block-4-polyvinylpyridine (PS-b-P4VP) was dissolved in tetrahydrofuran (THF), a common solvent for both the blocks, followed by spin coating the solution on silica/quartz substrate. It was then exposed to THF vapor for 30min in order to induce reordering of BCP micelles. Incorporation of metal oxide/metal NPs was done by subsequent dipping of the substrate in metaloxide/metal precursor solution for desired time, followed by oxygen plasma treatment, leads to the formation ZnO NWs decorated with silver or gold concurrent with partial removal of polymer. AFM was used to study the surface topography and the luminescence property was explored by using UV-Visible and photoluminescence instruments.

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Synthesis of Microporous Organic Molecular Networks by Cross-linking Polymerization of Tetrakis(4-isocyanatophenyl)methane and Various Amine Monomers

배재성, 박지웅

광주과학기술원 신소재공학과

Microporous organic molecular networks were synthesized by cross-linking polymerization of tetrakis(4-isocyanatophenyl)methane with diamines or tetraamines. By the sol-gel process, we were able to produce polymer solutions of the organic molecular network which enabled solution processable for practical application. The sol-gel processed organic molecular networks exhibited the microporosity and it defined by carbon dioxide adsorption and X-ray scattering (WAXS) data. Nanopaticles defined by dynamic light scattering(DLS), atomic force microscope(AFM), scanning electron microscope(SEM) and transmission electron microscope(TEM). We fabricated membranes by coating the network materials onto porous substrate.

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New 1-(2,6-diisopropylphenyl)-2,5-di(2-thienyl)Pyrrole-based Donor Polymers for Bulk Heterojunction Solar Cell Applications

V. Tamilavan, 현명호

부산대 화학과

A series of new donor polymers containing 1-(2,6-diisopropylphenyl)-2,5-di(2-thienyl)pyrrole namely PTPT, PPTPT and PTTPT have been synthesized and characterized. All three polymers have excellent solubility and thermal stability. The absorption spectrum of the all polymers covers the visible region from 300 nm to 600 nm. The optical band gap of PTTPT found to be ~ 2.13 eV, which is smaller than PTPT (~ 2.15 eV) and PPTPT (~ 2.20 eV). The polymers HOMO - LUMO energy levels are well matched for bulk heterojunction solar cell. The bulk heterojunction solar cells were made by the following configuration ITO/PEDOT:PSS/Polymers:PC70BM/TiOx/Al, active layer being sandwitched between holes injecting (PEDOT:PSS) and hole blacking (TiOx) layers. The effect of the addition of PC70BM in active layer was also studied. The surface of active layer was quite smooth; the root-mean-square (rms) roughness was found to be ~ 1.30 nm. The device made by PPTPT : PC70BM (1:5) as active layer showed the maximum power conversion efficiency (PCE) ~ 1.35% with current density (Jsc) of 7.41 mA/cm2, open circuit voltage (Voc) of 0.56 V and fill factor (FF) of 33%.

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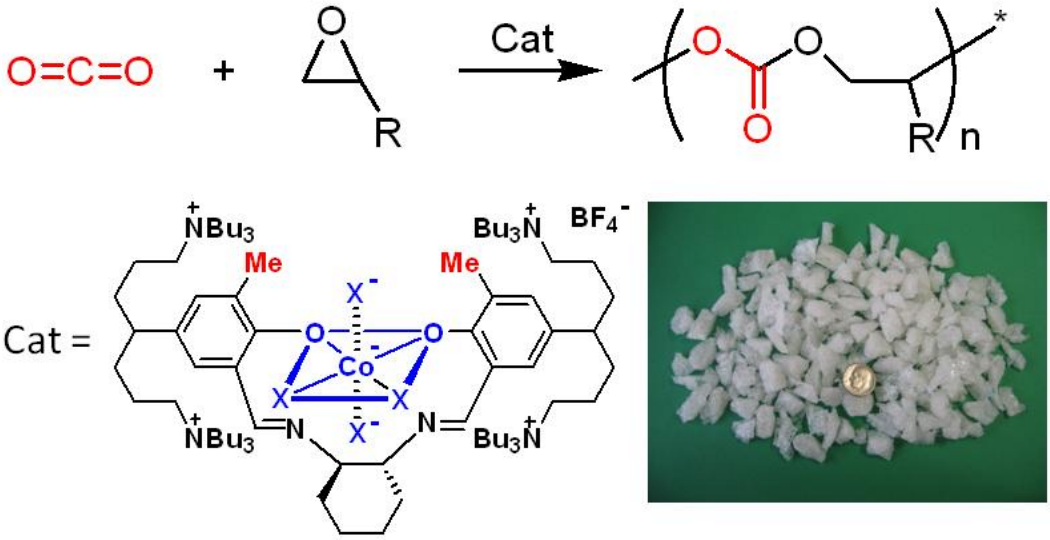
Elucidation of the Structure of a Highly Active Catalytic System for CO_2/EpoxideCopolymerization: A salen-Cobaltate Complex of an Unusual Binding Mode

Anish Cyriac

아주대 분자과학기술학과

Salen-type ligands comprised of ethylenediamine or 1,2-cyclohexenediamine, along with an salicylaldehyde bearing a methyl substituent on its 3-position and a -[CR($CH_2CH_2CH_2N^+Bu_3$)$_2$] (R = H or Me) on its 5-position, unexpectedly afford cobalt(III) complexes with uncoordinated imines. In these complexes, two salen-phenoxys and two 2,4-dinitrophenolates (DNPs), which counter the quaternary ammonium cations, coordinate persistently with cobalt, while two other DNPs are fluxional between a coordinated and an uncoordinated state in THF at room temperature. The complexes of this binding mode show excellent activities in carbon dioxide/propylene oxide copolymerization (TOF, 8 300-13 000 h^{-1}) but with some fluctuation in induction times (1-10 h), depending on how dry the system is. The induction time is shortened (¯). Imposing steric congestion either by replacing the methyl substituent on the salicylaldehyde with tert-butyl or by employing $H_2NCMe_2CMe_2NH_2$ instead of ethylenediamine or 1,2-cyclohexenediamine results in conventional imine-coordinating complexes, which show lower activities than uncoordinated imine complexes.



THE KOREAN CHEMICAL SOCIETY

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Conductive polymer photopatterning on flexible substrate from vapor polymerizable and photo cross-linkable EDOT

김정훈, 유정목, 김은경

연세대 화학공학과

We prepared a conductive polymer, PEDOT-MA, using vapor phase polymerization (VPP) method of 3,4-ethylenedioxythiopene with methacrylate end group (EDOT-MA) and photochemically induced a conductivity change of the PEDOT-MA film, to ensure a flexible conductive pattern. The room temperature conductivity (σ_{RT}) of the PEDOT-MA film on PET was 178 S/cm after doping. The conductivity of PEDOT-MA was decreased 99.97 % by photoirradidation due to the photo cross-linking of the methacrylate side chain. The photo cross-linking reaction of the side chain by photoirradiation using photomask and holographic method generated various pattern shapes and sizes which the light-exposed areas appeared as bleached and less conductive. Here, we report the study of conductive polymer patterning, effect of doping, conductivity mechanism under nanopatterns, and electronic diffraction.

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Characterization of selenious acid doped polyaniline: effects of dopant and water content

송예리, 이호익, 손대원

한양대 화학과

Among the intrinsically conducting polymer, polyaniline (PANI) has received considerable attention due to its unique chemical sensing and electrical properties. In this work, a simple and practical method to synthesize PANI nanostructures with selenious acid (SELA) as an effective dopant has been demonstrated. PANI has been synthesized by varying the dopant/monomer (D/M) mole ratio and it showed various morphologies such as nanospheres, nanorods and nanoflakes using only a dopant, without the use of a surfactant or template. In our research, with increasing D/M ratio, the crystalline degree of PANI is declined from 34% to 24%. It regards to the d-spacing of each PANI structure. The water content also decreases by D/M ratio which shows opposite change from an upward tendency of conductivity. Hence, control of water content will provide possibility for obtaining higher conductivity. We also found the relation between water content and PANI structure through XRD. TGA, UV-vis spectra and DSC.

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pH-sensitive organic/inorganic hybrid hydrogel for control release

전민희, 이호익, 손대원

한양대 화학과

Hydrogels are particularly useful in various applications as sensors, adsorbents, and materials in drug delivery systems as well as in solving some ecological and biological problems. Previously, we presented easy way of synthesizing hydrogel with organic/inorganic structure by gamma ray radiation. This hydrogel has a novel, pure network structure, high mechanical strength and pH-sensitive swelling effect. The swelling behavior of hydrogel depends on the reaction conditions such as the initiator content, initial monomer concentration, and cross-linker content. We test the swelling effect in gradient pH solution and various solvent. Our hydrogel can swell by 30～1000 times in various solvents due to the interaction between hydrogel and hydroxide ions. In the different polarity of solvents, we confirmed that the synthesized hydrogel is more swelled in large polar solvent. And in pH solutions, hydrogel is not swelled in acidic solutions (pH7).

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Synthesis and Characterization of Poly(oligothiophene)s

정은영, *박지웅

*광주과학기술원 신소재공학과,PIMS,RISE *광주과학기술원 신소재공학과*

The α,ω, - hydroxyalkyl substituted oligothiophene was synthesized by the Stille coupling reaction in the presence of $Pd(PPh_3)_4$. The oligothiophene were polymerized with diisocyanate or dicarboxylic acid monomers which can react with functional group of oligothiophene to produce polyurethane or poly ester. The resulting polymer had good solubility in common organic solvents. The structure of the polymer was studied by AFM and SAXS/WAXS. The thermal, optical and electronic properties of the polymer were investigated by TGA, DSC, UV-vis spectroscopy.

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Photocure Properties of New Type Photopolymer Systems with Organic-Inorganic Nano-hybrid Composite Materials

정대영, *김환건

*서경대 *서경대 응용화학과*

The new type organic-inorganic nano-hybrid photopolymers with photo-functional cinnamic group and inorganic siloxane moiety were synthesized to increase the heat resistant and transparency. These photopolymers can be performed photo-dimerization without photo-intiators, and have a network formation with siloxane unit through hydrolysis. The photo-cure reaction conversion of these systems with UV irradiation time were investigated using UV spectroscopy, and thermal stability and transparency with high temperature were measured by TGA and UV. Reaction rate constants with UV power in these systems were reported in terms of n-th order curing reaction equation. Excellent properties of thermal stability and transparency in these systems were observed, especially the best properties can be obtained in CA-S510.

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Functionalized Fullerene–Multiwalled Carbon Nanotube Composites for Bulk Heterojunction Photovoltaic Cells

정연수, 표명호

순천대 화학과

Organic photovoltaic cells (OPVs) are a promising low fabrication cost, lightness, simple fabrication process and flexibility than the silicon based solar cells. However these cells has a low power conversion efficiency, thus a great deal of effort is being devoted to increase the power conversion efficiency. Energy conversion efficiency of OPVs has been approaching 5% using conjugated polymer poly(3-hexylthiophene) (P3HT) as the electron donor and fullerene derivative (6,6)-phenyl-C61-butyric acid methyl ester (PCBM) as the electron acceptor. PCBM is effective in bulk heterojunction cells because of its high solubility in common solvent and efficient exciton dissociation. On the other hand, multiwalled carbon nanotubes (MWNT) are excellent at electron transport due to highly conductivity property. Moreover it has unique physical, mechanical properties. Therefore our object is to study the possibility of efficient charge separation at the polymer/functionalized fullerene interface followed by efficient electron transport through MWNTs to achieve best energy conversion efficiency. In this work, we describe the synthesis of fullerene-modified MWNTs and application in bulk heterojunction photovoltaic cells. The composites were made by first preparation of functionalized fullerene which was hydrolyzed with hydrochloric acid/acetic acid from PCBM. Then MWNTs with -OH group and coupling reagent added into the functionalized fullerene in common solvent. Photovoltaic cells were fabricated with fullerene-modified MWNTs and conjugated polymer P3HT. A fullerene-modified MWNTs were investigated by UV-visible spectroscopy (UV-Vis), photoluminescence (PL), fourier transform infrared absorption (FT-IR) and field emission scanning electron microscope (FE-SEM).

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Uneven surface structures in semiconducting polymer nanolayers made using micro/nano-pressing techniques

박지호, 김화정, 김영규

경북대 화학공학과

Semiconducting polymers have been extensively studied for optoelectronic device applications such as organic light-emitting devices, organic solar cells, organic field-effect transistors, organic memory devices, etc. Most of these conventional organic electronic devices employ a planar thin film (nanolayer) active layer, which has no particular features or structures on the layer (film) surface, sandwiched between electrodes. Recently we have attempted to make uneven surface structures on the nanolayer of semiconducting polymers by applying our patented micro/nano-pressing techniques. In this presentation we will discuss on the formation of particular uneven structures on the nanolayer surfaces and their structural features in detail. In addition, some examples of applications to organic electronic devices (solar cells) will be displayed.

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Cellular uptake efficiency using cell penetrating peptides modified silica particles

김희석, *신관우

*서강대 화학과 *서강대 화학과 및 바이오융합과정*

효과적인 유전자 전달 시스템을 위해서는 non-toxic carrier 의 선택과 표면 charge 의 제어가 필수적인 요소이다. 본 연구에서는 cell penetrating agents 로써 알려져 있는 HIV-1 TAT 단백질에서 얻어진 trans-activator factor 를 이용하여 표면 개질한 silica nanoparticles 를 다양한 크기 (50 nm ~ 800 nm)로 합성하여 세포내 투과의 효과를 연구하였다. 각각의 particle 은 FITC dye 가 particle 내부에 insertion 되었고 cellular uptake 후에 세포 내부의 형광 intensity 를 flow cytometry 및 형광현미경으로 비교 분석하였다. 큰 size (800 nm)의 particles 에서는 TAT 의 유무와 관계없이 대부분의 세포내에서 형광을 관찰할 수 있었지만 작은 size (200 nm)의 particle 에서는 TAT 표면 개질된 particle 의 경우, 약 두 배정도 많은 세포에서 형광이 관찰되었다. 또한 형광의 세기는 TAT 개질된 particle 이 개질되지 않았을 때 보다, 작은 particle 과 큰 particle 에서 각각 8 배와 3 배의 강한 형광을 관찰할 수 있었다. 이러한 결과는 TAT 단백질이 작은 size 의 particle 도 세포내부로 잘 전달할 수 있다는 것을 지시하고 있다. 추가적으로 100nm 이하의 더 작은 particle 에서도 delivery 효율 실험을 수행하고 있다.

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Two-component mixed SAMs gradient (methyl-carbonyl, methyl-amine, and carbonyl-amine) surfaces for the index of cellular adhesion properties

KHATUA DIBYENDU, *신관우

*서강대 화학과 *서강대 화학과 및 바이오융합과정*

Precisely controlled adhesion and growth of cells on biomaterial surfaces is a critical issue for successful development of biomedical devices and artificial organs. Among the surface properties, surface wettability and surface charges have been gained considerable attaintion, because these parameters have been found to affect critically the cell adhesion behaviors. Precisely controlled, widely varied surfaces are necessary for comparison the cellular behaviours. Self–assembled monolayers (SAMs) of alkylsiloxanes and alkanethiols have been considered as model surface for biological applications because they can form well-defined and stable surfaces.In this study, we have prepared two-component mixed SAMs gradient (methyl-carbonyl, methyl-amine, and carbonyl-amine) surfaces. The surfaces were characterized by contact angle measurements, X-ray photoelectron spectroscopy, and zeta potential measurements. We studied the adhesion behaviour of different types of cells on these surfaces and indexed each surface with respect to there surface properties for each type cells to sort them out depending on their adhesion properties.

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Fabrication of a microsieve network inside a fluidic channel as a platform for the miniaturized sample purification system

Lin Zhi Tang, *이내윤

*경원대 바이오나노학부 *경원대 바이오나노학과*

We introduce the fabrication of a microsieve network via photopolymerization directly inside a microchannel. The microsieve precursor solution is prepared by mixing UV-curable poly(ethylene glycol) diacrylate (PEGDA) with methacrylate-terminated silane reagent in predetermined ratio to ensure the formation of porous structure with free terminal Si groups. The fabrication scheme is based on the functionalization of the inner surface of a channel with silane coupling agent whose terminal group can react with the introduced microsieve precursor solution, followed by the reaction with tetramethoxysilane (TMOS) to supply sufficient Si functionalites at the terminal which can be adopted for the capturing of nucleic acid. In this research, the formation of porous microsieve networks are confirmed by fluorescence observation, and are adopted for nucleic acid purification purposes.

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Hydrogen Sensors Based on Chemically Synthesized Polythiophene Nanofibers

한승현, 신구, *L. Al-Mashat, *K. Kalantar-zadeh, *W. Wlodarski

*세종대 화학과 *RMIT University, Melbourne, Australia*

In this work, a comparative study on hydrogen gas sensors based on polythiophene nanofibers synthesized with two different oxidants is conducted for the first time. Polythiophene nanofibers have been synthesized through a template-free synthetic route and characterized using Scanning Electron Microscopy (SEM) as well as Ultraviolet-visible (UV-vis) and Fourier Transform Infrared (FTIR) spectroscopies. X-Ray Diffraction (XRD) studies in conjunction with the SEM data established the structural difference between the two nanofibers. Conductometric transducers were fabricated and used to measure the resistance of polythiophene nanofiber films during interaction with hydrogen gas at room temperature. It was found that the sensitivity of the sensor based on chloride doped polythiophene nanofibers was 1.363 towards 1 % of H2 gas. However the sensitivity of the sensor based on perchlorate doped polythiophene nanofibers was only 1.015 towards the same concentration of H2 gas. This difference in sensitivities between the developed sensors is directly related to the characterization data of the two nanofibers.

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Synthesis of Nanoporous Polyanilines and their Hydrogen Gas Sensing Properties

한승현, 신구, *L. Al-Mashat, *K. Kalantar-zadeh, *W. Wlodarski

*세종대 화학과 *RMIT University, Melbourne, Australia*

Novel layered Surface Acoustic Wave (SAW)/nanoporous polyaniline based hydrogen sensor has been developed. Nanoporous polyaniline is synthesized directly from anilium salts in a template-free reaction. Characterization of the synthesized nanomaterial was conducted through Scanning Electron Microscopy (SEM) as well as Ultraviolete-Visible (UV-vis) spectroscopy. The nanoporous polyaniline was deposited onto a layered ZnO/36° $LiTaO_3$SAW transducer for gas sensing applications. The sensor was exposed to various concentrations of hydrogen (H_2) gas at room temperature. The sensor response towards 1% of H_2 gas was a decrease in its operational frequency by 48.23 kHz. The sensor has a stable baseline and repeatable response.

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Magnetic studies of chitosan-gold nanoparticle composites

이창훈

조선대 응용화학소재공학과

Chitosan has been known to be representative biomacromolecules.

대한화학회 THE KOREAN CHEMICAL SOCIETY

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Observation of an unconventional crystalline structure in sodium alginates

이창훈

조선대 응용화학소재공학과

During the last decade, we have studied possible chain cissions of a sodium alginate either under an ultra sonification or an electron beam irradiation. Since chain cissions can generate various radical species, electron magnetic resonance spectroscopy was applied for detecting the radical species.

THE KOREAN CHEMICAL SOCIETY

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Study on the Magnetism of All organic composites

권영완, *이창훈, 최동훈, 진정일

*고려대 화학과 *조선대 응용화학소재공학과*

Room-temperature ferromagnetic materials are essential for magnetic storage and spintronic devices. For a long time, inorganic materials have been taking a leading position in ferromagnetism. Recently, great challenges have been made for room temperature or higher temperature ferromagnetic materials based on organometallic materials. Many types of organometallic compounds have been developed. Recently, diverse organic compounds have been synthesized expecting ferromagnetism, but none of them revealed any magnetic behavior at room temperature. In this presentation, I will discuss the magnetic properties of the composites with organic compounds/organic additives.

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Atomistic molecular dynamics simulation studies on the confined linear and ring polyethylene thin films

정철, 윤도영

서울대 화학부

The structural characteristics of confined linear, ring polyethylene(PE) melts and their blends on graphite(0001) surfaces have been studied by using atomistic molecular dynamics simulations at 509 K. Layered structures of linear and ring melts near graphite/polymer interfaces are characterized by monomer density distribution, trans probability of backbone torsion angle and order parameters as a function of distance from graphite surface. Adsorption of ring PEs with N = 100 on graphite surface is observed by the analysis of center of mass and radius of gyration distribution but it is not in case of linear PEs with same N. It is found that ring chains are segregated at the graphite/polymer interface and also vacuum/polymer interface if blended with linear chains. The population of rings near both interrfaces is calculated as a function of temperature to investigate the origin of the segregation.

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Fully Aliphatic Polyimides and their Nanoporous Thin Films

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

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

It is necessary to develop insulating polymers with low dielectric constants for achievement of high integration and speed in semiconductor. Polyimides have attracted much attention as insulating materials in the microelectronics industry because of their high thermal stability and excellent mechanical properties. In this work, aliphatic polyimides were prepared by two methods; one is commonly used two-step method and the other is a silylation method. Triblock polymers containing various amounts of thermally labile poly(propylene oxide) (PPO) block were prepared. Nanopores were introduced into the aliphatic polyimide by thermolysis of PPO block. Thin films prepared by the two-step method were brittle and pores with diameters of several hundred nanometer were formed, whereas, uniform closed nanpores were obtained by the silylation method. Structure of all prepared monomers and polymers was confirmed by 1H-NMR and FT-IR. The thermal properties of the polymers were investigated by thermogravimetric analysis (TGA) and differential scanning calorimetry (DSC). The pores were characterized by scanning electron microscope (SEM).

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Filtration of variously sized giant unilamellar vesicles using microfluidic chip

허유희, *신관우, **이기라

*서강대 화학과 *서강대 화학과 및 바이오융합과정 **충북대 공업화학과*

Giant unilamellar vesicle (GUV), consisting of single phospholipid membranes with diameters greater than 10 μm, are excellent biological models for dynamics and physical properties of many biological phenomena. Among various preparation methods of GUV, electroformation method, where external electric field is applied to lipid films deposited on an electrode, is commonly used to produce GUVs. However it is technically difficult to control the size of GUVs. Therefore, production of GUVs having various sizes seems to be inevitable. We recently designed a microfluidic chip, which could separate the smaller GUVs with diameter less than 10 μm which were mixed with the larger GUVs. In this presentation, we would like to present the chip design, and operation parameters (flow rate, channel width, and the number of filtering channels). We also tested the separation efficiency for GUVs made of different phospholipids. Since elasticity and stability of GUVs, depending on the phospholipids, are very different, we expect that the separation efficiency might be very different.

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DSSC Based on Polythiophene Derivatives

조연경, 표명호

순천대 화학과

DSSC 는 다른 photovoltaic cell 에 비해 공정이 단순한 반면 상대적으로 높은 효율을 갖기 때문에 특정 용도로 응용 가능성이 기대되고 있다. DSSC 에 가장 일반적으로 사용되는 Ru complex 는 가시광선 영역에서 IPCE 가 80%에 이르는 등 높은 초기효율을 보이나, dye 의 가격이 높고 NIR 흡광이 제한적이다. 이에 반해 conjugated polymer(CP)는 높은 몰흡광 계수와 광범위한 흡광 영역 때문에 precious metal-containing dye 의 substitute 로 많은 관심을 모으고 있다. 또한 CP 는 구조를 변형시키는 것이 용이하며, 다양한 유기 용매에 녹을 수 있는 장점을 가지고 있다. CP 중 가장 폭넓게 연구되고 있는 polymer 는 thiophene 계로서, S. Yanagida 등은 poly(3-thiophene acetic acid) dye 에 imidazolium salt 를 사용하여 2.4%의 효율을 얻었다고 보고하였다. 본 연구에서는 3-thiophene acetic acid(TAA)와 thieno[3,4-b]thiophene-2-carboxylate(TTEt)의 homo 또는 co-polymerization 을 통하여 얻은 polymer 를 DSSC 용 dye 로 이용하여 panchromatic DSSC 를 제조하는 실험을 수행하였으며, dye 의 높은 분자량으로 인해 TiO2 film 의 porosity 가 증가함에 따라서 효율이 증가하는 것을 확인하였고, 크기가 다른 두 종류의 TiO2 조성 비율에 따른 효율 변화를 측정 하였다. 또한 가시광선 영역뿐만 아니라 NIR 영역까지 흡광 영역을 넓히기 위하여 homopolymer mixture 또는 copolymer 를 dye 로 이용한 DSSC 의 성능을 비교하였다.

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On-Demand Theranostic Applications of Hyaluronate-Cucurbituril Conjugate

정현태, *박경민, **양정아, 이돈욱, ***류성호, ****한세광, *****김기문

*포항공과대 시스템생명공학부 *포항공과대 첨단재료과학부 **포항공과대 신소재 공학과 ***포항공과대 분자생명과학부 ****포항공과대 신소재공학과 *****포항공과대 화학과*

Polymeric systems have been developed to deliver drugs directly to the intended site of action and also to improve efficacy while minimizing unwanted side effects elsewhere in the body. However, they often require complicate, time-consuming chemical synthesis for conjugation of functional tag molecules such as imaging probes, aptamers, functional moieties, and drugs. It is also possible that biomolecules conjugated to polymer backbone can be damaged or deactivated their functions under the repeated chemical reactions. Cucurbit[6]uril (CB[6]), a member of the macrocyclic host family cucurbit[n]uril (CB[n]), forms stable host-guest complexes with polyamines with extremely high binding affinity (K > 107 M-1) in aqueous solution. Here we present a multifunctional delivery platform based on host-guest chemistry using hyaluronate, a biodegradable, biocompatible polymer. Functional tag-attached spermidine conjugates such as FITC-spmd and peptide-spmd can be introduced on the HA-CB[6] conjugate without losing their functions, suggesting that the HA-CB[6] conjugate can be used as a supramolecular chemistry-based multifunctional delivery platform for on-demand theranostic applications.

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in situ formation and modification of hydrogel using sequential host-guest interactions: a noncovalent and modular approach to provide three-dimensional cell environments

박경민, *양정아, **정현태, ***한세광, ****김기문

*포항공과대 첨단재료과학부 *포항공과대 신소재 공학과 **포항공과대 시스템생명공학부 ***포항공과대 신소재공학과 ****포항공과대 화학과*

In situ-forming hydrogel has been studied for three-dimensional (3D) cell culture to understand the role of 3D physical and chemical environments in cell function, as well as regenerate tissue structures. However, the processes for preparation and modification of hydrogels often cause severe cytotoxicity, since most *in situ*-forming hydrogels are formed by chemical cross-linking using additional chemical reagents with stimuli such as temperature changes or UV irradiation. Cucurbit[6]uril (CB[6]) is a synthetic macrocyclic molecule that forms stable host-guest complexes with polyamines with high binding affinity ($K > 10^7 M^{-1}$) in aqueous solution. Using the strong host-guest interactions, we present here a versatile, biocompatible *in situ*-forming hydrogel that can be readily prepared and further modified in a noncovalent and modular manner. The hydrogel was formed by simple mixing of CB[6]-attached hyaluronic acid (HA) conjugate (CB[6]-HA) and 1,6-diaminohexane(DAH)-attached HA conjugate (DAH-HA) not only in vitro but also in vivo. Additionally, we observed enhanced attachment of preosteoblase cells in the hydrogel in which RGD(Arg-Gly-Asp)-attached CB[6] was noncovalently introduced using host-guest chemistry. This supramolecular approach to form and modify the hydrogel can thus provide a novel method for a versatile and biocompatible biomaterial platform.

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Cross-linked Organosilicate Hole Transporting Layers for Organic Optoelectronic Devices

강예랑, *윤도영, **Alla Sellinger

*서울대 화학 *서울대 화학부 **Stanford University*

The integrity of interfacial contact between inorganic indium tin oxide (ITO) anode and organic layer is crucial for the performance in organic optoelectronic devices. In order to resolve the shortening of conventional PEDOT:PSS hole injection/tansporting layer (HITL), a novel organosilicate polymer based on N,N'-diphenyl-N,N-bis(4-E)-2(triethoxysily)vinyl)phenyl)biphenyl-4,4'diamine was synthesized and characterized. Insoluble HITL was prepared via spin-coating of soluble prepolymer and subsequent thermal crosslinking. Electrochemical and optical properties of the new hole transporting material have been characterized, and the device performances of solution-processed polymer light emitting diodes (PLEDs) and organic photovoltaic cells have been investigated.

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Influence of costabilizer in mircoencapsulation of paraffin wax

강길준, *김성훈, **조창기

*한양대 섬유고분자 공학과 *한양대 섬유고분자공학과 **한양대 응용화공생명공학부*

Microcapsules are composed of polymer shell and active core with the size of 50nm to 2,000um. Size of microcapsule using miniemulsion can be smaller than 1μm. Miniemulsion is generally consists of oil, water, surfactant, and cosurfactant. In the miniemulsion, oil droplets are stable even though the size is smaller than 1um because of cosurfactant. In this work, polystyrene was used for encapsulation of paraffin wax. Generally, cosurfactant is very in-soluble in the water. Hexadecane, cetyl alcohol, stearic acid , and stearyl methacrylate are usually used as cosurfactant. In the encapsulation of paraffin wax, cosurfactant is not necessary. Because paraffin wax can act as the costabilizer. The size of the obtained nanoparticles was measured by dynamic light scattering.

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Characterization of microcapsule prepared by using buffer solution

김성훈, *강길준, **조창기

*한양대 섬유고분자공학과 *한양대 섬유고분자 공학과 **한양대 응용화공생명공학부*

Microcapsules are fine particles whose size ranges from 50nm to 2,000 ㎛, composed of polymeric shell and active core component. Microcapsules containing phase change materials(PCMs) were successfully prepared by in situ polymerization using melamine-formaldehyde(MF) resin as the shell and n-octadecane as the core. MF prepolymer was prepared in the alkaline condition, and mixed with octadecane emulsion for encapsulation. Encapsulation was controlled by pH through buffer solution. The range of phosphate buffer for this study is generally from pH 5.5 to 8.5. In this study, properties of microcapsule were analyzed in terms of the pH of buffer solution and concentrations.

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A study of cross-linked copolymer membrane for PEMFC containingsulfonated poly(ether sulfone) and poly(p-phenylene terephthalamide) segments

김정민, *조창기

*한양대 섬유고분자공학과 *한양대 응용화공생명공학부*

Aromatic polyamides have thermal stability and high strength, make themselves attractive in many applications. However, their processability is quite limited due to hydrogen bonding, poor solubility in common organic solvents, and the high melting points. In order to improve the processability, other co-segments can be incorporated into the polymer chain. In this study, copolymers containing sulfonated poly(phenylene ether sulfone) and p-phenylene terephthalamide were prepared to check the possibility as membrane materials for fuel cell application. Prepared copolymer membranes were characterized in terms of the proton conductivity, ion exchange capacity (IEC), water uptake, methanol permeability, and thermal stability. Detailed results will be presented.

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Preparation of Anion Exchange Membranes by Amination of Poly(Vinylbenzyl Chloride)-grafted FEP Films

신준화, *고범석, 노영창

*한국원자력연구원 정읍방사선과학연구소 *전북대 방사선과학기술학과*

Poly(vinylbenzyl chloride)-grafted FEP (poly(tetrafluoroethylene-co-hexafluoropropylene) films prepared by a radiation grafting method utilizing γ-ray were utilized for the preparation of anion exchanging membranes (AEMs), in this study. The reaction conditions for the amination of the grafted films with various amines such as trimethylamine, N,N-dimethylbuthylamine, N,N-dimethylaniline N-dimethylpiperidine were optimized. The ion exchanging capacity (IEC), water uptake (WU), thermogravimetry analysis (TGA), and mechanical property of the prepared membranes were also investigated and the results are reported in this presentation.

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Photoreactive main chain conjugated polymer containing oxetane moieties in the side chain and its application to green electrophosphorescence devices

신지철, 이태완, 김경환, 최동훈

고려대 화학과

The utilization of a photoreactive hole injection/transport layer in multilayer electrophosphorescence polymer light-emitting diodes (PLEDs) is demonstrated in this study. A new photoreactive polymer was synthesized using 3,6-dibromo-9-(6-((3-methyloxetan-3-yl)methoxy)hexyl)-9H-carbazole and 2,4-dimethyl-N,N-bis(4-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)phenyl)aniline via the Suzuki coupling reaction. When oxetane groups were photopolymerized in the presence of a cationic photoinitiator, the cured film showed good compatibility with PEDOT:PSS and the indium tin oxide (ITO) layer due to the hydrophilic nature of the cross-linked section. The resulting green lightemitting device bearing PVK:PBD:Ir(Cz-ppy)3 exhibits a maximum external quantum efficiency of 8.73%, corresponding to a luminous efficiency of 28.2 cd/A when using the device configuration of ITO/POx-TPACz/PEDOT:PSS/PVK:PBD:Ir(Cz-ppy)3/TAZ/Alq3/LiF/Al. These values are higher than those of PLEDs using conventional PEDOT:PSS as a single hole injection layer (HIL). The slight degree of improvement in device efficiency is due to the reduced hole injection barrier.Our study unambiguously describes a new POx-TPACz interlayer that takes advantage of efficient hole transport and solvent resistance. It can be fully utilized for fabricating better solution proceed phosphorescent EL devices

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Analysis of the Wettability of Partially Fluorinated Polymers Reveals the Surprisingly Strong Polar Character of Poly(vinylidene Fluoride)

이상화

경원대 화학생명공학과

The wettabilities of the partially fluorinated polymers (ethylene-tetrafluoroethylene copolymer (ETFE), ethylene-chlorotrifluoroethylene copolymer (ECTFE), and poly(vinylidene fluoride) (PVDF)) were investigated by contact angle measurements. Zisman plots for ETFE and ECTFE exhibited linear relationships, while the Zisman plot for PVDF showed a slight curvature, which was interpreted to indicate strong non-dispersive interactions between the surface and the contacting liquids. The Lifshitz-van der Waals forces of the fluoropolymers were estimated to increase in the order of ETFE < PVDF << ECTFE. An evaluation of the polar or "acid-base" interaction energies showed that PVDF, which possesses the most acidic hydrogens among the examined fluoropolymers, has the strongest non-dispersive interactions.

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Organically Functionalized DNAs and their Application to the Bio-organic Field Effect Transistors

김윤선, 김경환, 이태완, 진정일, 최동훈

고려대 화학과

Recently, DNA has been studied electronic, photonic, and magnetic properties. Those are utilizable in such advanced technologies as bio-organic field effect transistors (BioFET), bio-organic light emitting diodes (BioLED), nanowire, template, optomagnetic switching, and molecular magnetic information storage. The purified natural DNA can be dissolved only in water, but not soluble in any other organic solvent. In this study, we modified the structure of natural DNA and change its solubility by post-functionalization. We applied organically functionalized DNAs to electronics and optoelectronics. The organic soluble DNA contains chalcone moiety which is photoreactive was utilized as a gate insulator for BioFET. We fabricated TFT device using organic semiconductor material and the photocrosslinked DNA-based gate insulator by solution deposition method. The device performances will be demonstrated in this presentation.

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π-Conjugated Molecules based on Anthracene Derivatives bearing a thienothiophene moiety as Organic Semiconductors

조소영, 배숙영, 김경환, 최동훈

고려대 화학과

Interest in organic semiconductors has increased in recent years due to potential applications in optoelectronic devices such as organic thin-film transistors (OTFT). In the solid state of organic semiconductors, the intrinsic carrier mobility depends critically on the degree of molecular orientation and on the extent of the intermolecular interaction. In this study, X-shaped conjugated molecules were synthesized. Allyl-substituted aromatic peripheral moieties into an anthracenyl core improve the solubility in organic solvent for the solution-based device fabrication. They display a p-type semiconducting behaviors and their electrical properties are investigated in detail. We performed the UV-visible absorption spectroscopy, photoluminescence spectroscopy, cyclic voltammetry, and thermal analysis of the new π-conjugated molecules. Finally, we fabricated thin film transistor to investigate the device performances.

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NIR-Fluorescent Dye Embedded PEGylated Block Copolymer

허정아, 신지철, 조소영, 김경환, 최동훈

고려대 화학과

There has been increased interest in the use of polymeric micelles as carriers for near-infrared fluorescence (NIRF) dyes for a cancer diagnosis. In polymeric micelles, fluorescent dyes are effectively incorporated in the cores of micelles. In addition water-dispersed functional micelles are attracting considerable interests in biological and biomedical application. Although various approaches have been reported for the dispersion of micelles in water, it remains challenge to develop a general method to stabilize disperse micelles in aqueous media. We first synthesized amphiphilic block polymers by atom transfer radical polymerization. When the amphiphilic polymer and dyes were dissolved together in organic solvent, the addition of water caused the spontaneous formation of polymeric micelles, resulting in the successful encapsulation and aqueous dispersion of micelles. The properties of the resulting core-shell micelles were investigated in detail.

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Self-organization of X-shaped π-Conjugated Molecules based on Anthracene Derivatives and their Application to Thin Film Transistors

배숙영, 김경환, 최동훈

고려대 화학과

Organic semiconducting materials based on π-extended linear-conjugated systems have been very intriguing and significant development has been achieved in these materials over the one decade. In the exploration of the application as organic semiconductors in organic thin film transistor (OTFT) is an important component for developing future flexible displays. In organic semiconductors, the intrinsic carrier mobility depends critically on the degree of molecular orientation and on the extent of the intermolecular interaction. In this presentation, new crystalline X-shaped conjugated molecules will be demonstrated. Introduction of thiophene-based peripheral moiety into an anthracene core improve the solubility in organic solvent for facilitating the solution device fabrication. They showed intriguing mesoscopic self-organization of molecules inducing the anisotropic alignment. We investigated the photophysical and electrical properties of the new X-shaped molecules. Finally, we fabricated thin film transistor to investigate the carrier mobility.

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Synthesis and characterization of photoreactive multi-branched semiconducting molecules and containing an anthracene central moiety

하재승, **Hoang Mai Ha**, 이태완, 김경환, 최동훈

고려대 화학과

Organic semiconductor materials have been very intriguing and significant development has been achieved in the past years. The development of organic field effect transistors (OFETs) has generated a great deal of interest in the availability of solution processible organic semiconductors, which can combine high charge transport mobility, stability and patternable. In this work, we synthesized photoreactive-conjugated X-shaped molecules and characterized their physical properties. The solubility of molecules was found very good for solution processing. The photopatterning of organic semiconductor was carried out by photocrosslinking reaction of the reactive end groups, resulting in a crosslinked 3-D network. These molecules display a p-type semiconducting behavior and their electrical properties are investigated in detail.

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Synthesis and Characterization of New Donor-Acceptor Type Copolymer for Polymer Solar Cell Applications

이태완, Hoang Mai Ha, 김경환, 최동훈

고려대 화학과

The concept of internal electron donor–acceptor (D–A) interaction has been extensively exploited to prepare low band-gap organic semiconductors. Using this strategy, new low band-gap materials have been developed to expand the absorption spectrum to NIR range. In addition, it is generally accepted that the formation of strong intermolecular $\pi - \pi$ stacking is necessary to achieve high charge mobility in organic semiconductors. Introduction of rigid coplanar fused aromatic rings efficiently enhance intermolecular interaction and hence improve charge carrier mobilities. Therefore, the copolymers consisting of an electron-accepting benzothiadiazole-cored thiophene and an electron-donating heteroarenes have been designed and synthesized. We expect this polymer would have narrow band-gaps and high charge carrier mobility owing to the large fused heterocyclic aromatic ring of thiophene, benzothiophene and the D–A structure in the polymer backbone. Polymer solar cells were fabricated and their performance was characterized.

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Self-assembled semiconducting monolayer prepared with 5,5'-(9,10-bis((4-hexyl phenyl) ethynyl)anthracene-2,6-yl-diyl)bis (ethyne-2,1-diyl)bis(2-hexylthiophene) based trimethoxysilane

이주빈, 김윤선, 이태완, 김경환, 최동훈

고려대 화학과

Recently, we reported very interesting semiconducting properties of anthracene based conjugated molecules, investigated in thin film transistors. The anthracene moieties demonstrated quite unique molecular aggregation and strong intermolecular interaction in the solid state. From this motif, we prepared trimethoxysilane bearing the corresponding semiconducting moiety as a precursor molecule for elaborating self-assembled monolayer(SAM) on the hydroxyl functionalized substrate. The absorption and emission properties of SAM were compared with those of solution and bulk films. With the deposition condition, the density of semiconducting molecules and the packing structures were investigated using atomic force microscope and confocal fluorescence microscope. Finally, the monolayer was inserted between silicon oxide gate insulator and organic semiconductor in thin film transistors. The device performances were characterized in detail.

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New conducting Polymer Containing Carbazole Derivative, Benzothiadiazole and EDOT in the Main Chain

한우택, 김인태

광운대 화학과

New polymer Containing Carbazole Derivative, Benzothiadiazole (BT) and EDOT, Ethylene were synthesised by stille reaction. The resulting polymer was showed excellent solubility in common organic solvents, such as dichloromethane, chloroform, toluene, and THF. The characterization of the copolymer was measured by ^{1}H-NMR, ^{13}C-NMR, FT-IR, UV-vis and PL. The molecular weight of the copolymer was measured by GPC. Themal properties of copolymer was investigated by TGA. The application of the new polymer as emitting layer in LED will be discussed.

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Synthersis and Optical Properties of Cyclopentadithiophene-Based Copolymer which Containing Electron Deficient Unit for Organic Photovoltaic Cell Applications

한우택, 정주희, 황선우, 김인태, 이상우

광운대 화학과

The Cyclopenta[2,1-b:3,4-b']dithiophene, the two thiophene units are confined to one plane, which prolongs the effective conjugated length of the polymer and effectively lowers the band gap. Futhermore, the two alkyl side chains on the CPDT unit give the polymer its excellent solubility, which is important for the formation of uniform films by the spin-coating process. Herein, we synthesized new conjugated copolymer containing coplanar CPDT units. The resulting copolymer was characterized by ^{1}H NMR, ^{13}C NMR, GPC and TGA. Electochemical and optical experiments of the resulting copolymer were observed by Uv-vis spectroscopy, PL spectroscopy and cyclovoltammetry. The resulting copolymer will be developed for the applications of polymer solar cells(PSCs).

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Anthracene-based Crack Sensor

조예현, 조성열, 정찬문

연세대 화학과

The purpose of this study is to develop an intelligent polymeric material by which microcracks are detected by its fluorescence change. Anthracene and its derivatives have been studied widely in the field of photochemistry. Dimers of 9-anthracenealdehyde (AA) and 9-anthracenecarboxylic acid (ACA) were synthesized by photoreaction via [4+4] cycloaddition. Cross linked polymers, Poly-AA and Poly-ACA were synthesized using PVA and the dimers as a crosslinking agent. Poly-Auth-AA and Poly-Auth-ACA were synthesized using PVA and the monomers, AA and ACA.Poly-AA, Poly-ACA and their ground samples were investigated by UV-Vis spectroscopy, FT-IR spectroscopy, photoluminescence spectroscopy and absolute quantum yield measurement. The IR spectra of ground Poly-AA and Poly-ACA were similar to Poly-Auth-AA and Poly-Auth-ACA respectively. The crosslinked polymers and their ground polymers showed a large difference in their fluorescence properties. Fluorescence microscopic images of microcracks in the anthracene-type polymeric material were obtained. In this study, it was demonstrated that the anthracene-based polymers could be used as a crack sensor.

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New Semiconducting Multi-branched Conjugated Molecules based on π-Extended Triphenylene for Electronic and Optoelectronic Applications

Hoang Mai Ha, 김경환, 이태완, 최동훈

고려대 화학과

Triphenylene derivatives are the most well-known representatives of discotic liquid crystals forming columnar mesophases. In this work, the authors report on the design and synthesis of a new class of semiconducting materials, based on a triphenylene core, those are solution processable. These molecules showed relatively low bandgap energies and interesting LC properties. These molecules have a good solubility and are applicable to soluble processing for organic field effect transistor (OFET). Their thermal stabilities and dynamic behaviours are suitable for OFET device fabrication. The findings reported in this paper are expected to contribute to the design of new discotic LC semiconductors based on π-extended triphenylene for future electronic and optoelectronic applications.

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Facile Method for Fabricating Superhydrophobic Surface

한문희, 안용현

단국대 화학과

Wettability is controlled by both the geometrical structure of a surface and a low surface energy material coating. A super-hydrophobic surface is satisfied with a water contact angle of more than 150° and a sliding angle of less than 10°. The nickel cluster deposition on Mg plate was obtained by using nickel sulfate and hydrazine hydrate. The modified magnesium plate was immersed in stearic acid in ethanol solution for 40min. The coated stearic acid was identified with XPS. The surface morphology of modified Mg plate was analyzed with SEM and super-hydrophobic properties of surfaces were determined by water contact angle measurement. We studied the relationship between pH and contact angle on superhydrophobic surfaces.

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Inkjet printed BHJ film morphologies for efficient organic solar cell

이의진, *이상호, **이재관

*한국생산기술연구원 융복합생산기술연구부 *한국생산기술연구원 융합생산기술연구부 **호서대 융합기술연구소*

Polymer solar cells and bipolar field effect transistor based on bulk-heterojunction (BHJ) materials comprising p-conjugated polymers and fullerene derivatives have attracted considerable attention over the past decades because of their unique advantages, such as low cost, lightweight, solution processibility, and flexibility. Thus, enormous efforts have focused on improving the device performances though developments of efficient materials and functional layers with providing a promising efficiency of 6% recently.1-15 Nevertheless, a general printing method such as spin-casting in laboratory may be strongly imposed restriction on production of large size patterned device as well as on a large expenditure of expensive materials for future commercial application. Therefore, some processing approaches using versatile printing technique such as doctor blade, inkjet, and roll-to-roll for fabrication of large area film in organic electronics, LED, FET, solar cell have emerged from the interest of scientific and engineering researches. An inkjet printing among these techniques has been extensively demonstrated with attractive advantages regarding high registration accuracy of direct writing in targeted active area without unnecessary waste of functional materials.Recently, Hoth et al. has reported an about 3% of inkjet (DimatixTM) printed organic bulk heterojunction solar cell using P3HT:PCBM composite in mixed ink solution of 68% of ortho-dichlorobenzene (oDCB) and 32% of mesitylene. However, although a high boiling ink formulation with oDCB or its mixed solvent was irresistibly applied to prevent nozzle clogging of the printhead, its use seems to be hard to control the morphology of BHJ film on top of PEDOT:PSS underlayer compared to that spin-cast. Herein, we wish to report that direct writing of P3HT:PCBM composite in BHJ solar cell can be efficiently addressed by inkjet printing technology using conventional chlorobenzene ink solution.

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Thermal Crack Healing in a Perfluorocyclobutane-Containing Polymer.

유미란, 조성열, *김중곤, 정찬문

*연세대 화학과 *한화석유화학(주) 바이오연구센터*

The object of this study is to develop an intelligent polymeric material for the crack self-healing. It is the polymeric materials for crack healing which can be readily healed by thermal cycloaddition. Perfluorocyclobutane (PFCB)-contaning 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 thermally mendable material was investigated. A healing agent, 1,1,1-tris(4-trifluorovinyloxyphenyl)ethane (TVE) for thermal healing was synthesized, and its chemical structure was confirmed by NMR and FT-IR spectroscopy. The polyTVE having perfluorocyclobutane was synthesized by thermal polymerization. Cracks were generated in polyTVE specimens, and a part of the cracked samples were heated to induce thermal healing reaction. The thermal crack-healing ability of a polyTVE was investigated by FT-IR spectroscopy. The crack healing in polyTVE was successfully demonstrated by the measurement of flexural strength of poly TVE specimens before and after healing.

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Preparation and Properties of Waterborne Polyurethane-silane: A Promising Foul Release Coating

Mohammad M. Rahman, 박현

부산대 첨단조선공학연구센터

Waterborne polyurethane-siloxane (WBPUSi) resins were prepared through a pre-polymer process using N-[3-(Trimethoxysilyl)propyl]-ethylenediamine (TMSiP-EDA). The TMSiP-EDA amine group reacted with NCO group of NCO-terminated prepolymer and the methoxy group made branching in two chains with Si-O-Si by hydrolysis and condensation reaction in water dispersion. The thermal stability and tensile strength of synthesized resins significantly improved comparing to those for conventional WBPU. A selected WBPUSi-resin was used to foul release coating to protect the marine fouling. The foul release property of the resin was examined during exposure to a marine environment after immersion for three months. The improvement to protect marine fouling was observed in WBPUSi.

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Fluorescence image patterning based on *o*-hydroxycinnamate derivates

송영규, 조성열, *김중곤, 정찬문

*연세대 화학과 *한화석유화학(주) 바이오연구센터*

Patterned fluorescent images are applicable in displays, optical memory devices, sensors and imaging industries. In this study *o*-hydroxycinnamates were prepared and their photochemical conversion into coumarins was utilized in fluorescence imaging.Four *(E)-o*-hydroxycinnamates were readily synthesized from salicyladehydes, and it was confirmed by ^{1}H NMR spectroscopy that the cinnamates photochemically converted into their corresponding coumarins via *(Z)-o*-hydroxycinnamate intermediates.The photoconversion was greatly accelerated in the presence of *p*-toluenesulfonic acid. However, when *p*-toluenesulfonic acid is used, the patterned images were somewhat unstable. Stable fluorescent images could be obtained by using triphenylsulfonium triflate.The optical properties of the cinnamates were compared with those of the corresponding coumarins. Fluorescence imaging was successfully accomplished by photoirradiation of PMMA films containing the cinnamates.The photoconversion of *(E)-o*-hydroxycinnamates is promising for the application to fluorescence imaging because there is no necessity for any additional processes such as wet developing and post-exposure bake, coupled with the ease of synthesis of the precursors.

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Synthesis of PEDOT in polycarbonate membrane in magnetic ionic liquid and its characteristics

김방한, 이미희, 오응주

명지대 화학과

In this study PEDOT was synthesized in polycarbonate membrane in magnetic ionic liquid (MIL) to obtain the polymer chain well ordered. SEM, TEM, IR spectrum, conductivity were measured to check the structure and properties of PEDOT synthesized. The results were compared with those of PEDOT synthesized in MIL only. Effect of synthetic condition on the properties of PEDOT will be discussed.

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Synthesis and Characterization of Low-Band-Gap Chromophores Containing π-Conjugated Triphenylamine-based Donor and Benzothiadiazole Acceptor through single, double and triple bond for Dye-Sensitized Solar Cell

이명준, *이동현, *송해민, *주명종, *김환규

*고려대 소재화학과 *고려대 신소재화학과*

A series of new π-conjugated metal-free organic dyes (TBC-S, TBC-D and TBC-T) comprising triphenylamine (TPA) moieties as the electron donor and benzothiadiazole moieties as the electron acceptor/anchoring groups were designed and synthesized for application in dye-sensitized solar cells (DSSCs). Triphenylamine units are bridged to benzothiadiazole with single(S), double(D) and triple bonds(T) in different derivatives. Their structure-property relationship has been investigated through the photophysical and photoelectrochemical studies. Under the photovoltaic performance measurement, a maximum photo-to-electron conversion efficiency of 5.71% was achieved with the DSSC based on dye TBC-S (Voc=582mV ,Jsc=15.01Ma/cm^2, ff=0.65) under AM1.5 irradiation of 100mWcm^{-2}.

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Cell Internalization of Oligopeptide into Osteoclast: Mechanism Study

Chi Bo, SHINDE USHA PRAMOD, 정병문

이화여대 화학나노과학과

Histidine and amine functionalized β-cyclodextrin were synthesized for the delivery of model drug into primary osteoclast precursor cells (bone marrow macrophages). By formation of inclusion complexes with cationic modified β-cyclodextrin, the hydrophobic model drug was successfully solubilised in aqueous solution. To investigate the cellular uptake of the inclusion complex, a series of inclusion complex was prepared with different molar ratio (1:0, 7:3, 5:5, 3:7 and 0:1) between of histidine modified β-cyclodextrin and amine modified β-cyclodextrin. Flow cytometry and spectrofluorimetry analysis indicated that the model drug itself was not taken up by the cell, however, inclusion complex systems underwent significant cellular uptake. In particular, inclusion complex formed by mixture of histidine modified β-cyclodextrin and amine modified β-cyclodextrin with a molar ratio 7:3 were taken up more efficiently than others. The mechanism of the cellular uptake of oligopeptide was also investigated using different celluar uptake inhibitors and accelerator. Cell viability study showed that both amine and histidine modified β-cyclodextrin exhibited no significant cytotoxicity.

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Synthesis and Characterization of Swivel- like anthracene based H-shaped Conjugated molecules

김경환, 최동훈

고려대 화학과

Oligo- and polythiophenes have recently received increasing attention because of their large field of application such as energy storage and electrochromic devices. One of the important areas where thiophene-based π-conjugated oligomers and polymers have been widely applied is as semiconductors in organic field-effect transistors (OFETs). In the exploration of the application as organic semiconductors in organic field effect transistor (OFET) is an important component for developing future flexible displays. Organic photovoltaic cell is also promising candidate device for future energy resources. In organic semiconductors, the intrinsic carrier mobility depends critically on the degree of molecular orientation and on the extent of the intermolecular interaction. In this study, Swivel-like anthracene based H-shaped conjugated molecules have been synthesized through the stille coupling reaction. They display p-type semiconducting behaviors and have much better solubility than the linear conjugated oligothiophene. We performed absorption spectroscopic analysis, electrochemical analysis, and PL spectroscopy.

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Effect of polyaniline on resistivity-temperature behavior of polyurethane / carbon black composite.

이상범, *박희수, *오응주

*명지대 전도성 고분자 연구실 *명지대 화학과*

To avoid the negative temperature coefficient (NTC) effect in the polyurethane (PU) / carbon black (CB) composite, the homogeneity of dispersion of CB should be improved. In this study CB was coated with polyaniline prepared by in-situ polymerization of aniline. The result of PTC intensity and the reproducibility of resistivity-temperature curve in heating / cooling cycles of polyaniline coated CB was compared with those of CB filled polyurethane composite. In the measurement of PTC/NTC curve, a digital multimeter and programmable oven was used. The degree of aggregation of polyurethane / CB and polyurethane / CB-PANI composites was compared from SEM image. The effect of synthetic condition to the resistivity-temperature characteristics will be discussed.

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Er(III)-cored Complexes Based on Boradiazaindacene(BODIPY) Ligands for Optical Amplifications : Synthesis, and Photophysical studies

유정호, 엄유경, *오정환, **송복주, 김환규, ***Jean-Claude G. Bünzli

*고려대 신소재화학과 *고려대 소재화학과 **고려대(세종) 신소재화학과 ***École Polytechnique Fédérale de Lausanne (EPFL), switzerland*

In recent fiber optic telecommunications, erbium-doped fiber amplifiers (EDFA) have been utilized in long distance fiber communication systems. Most of the rare-earth doped materials used so far have been prepared by doping rare-earth ions into inorganic glasses. In these systems, it is not possible to obtain the amplication gain of higher than 30 dB/cm, due to the poor solubility of the rare-earth ions into inorganic glasses, aggregation or phase separation and ion-ion interactions. To overcome these problems, we have designed and synthesized the highly efficient light-harvesting integrated materials. BODIPY dyes were prepared by the functionalized pyrrole, methyl 4-formylbenzoate and BF3OE, which would increase the shielding of the encapsulated lanthanide ion and the efficiency of the intramolecular energy transfer from suitable host materials to lanthanide ion. In this presentation, the synthesis and photophysical properties of the highly efficient light-harvesting integrated materials will be discussed.

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pH/Temperature Sensitive Thermal Gelation of Polypeptide Aqueous Solution

장지혜, 정병문

이화여대 화학나노과학과

Recently, much attention has been paid to stimuli-responsive polymers that can reversibly to small changes in environment, thereby resulting in a large change of physical property. Those stimuli-responsive systems are of interest in biomedical and pharmaceutical area. In this research, we introduced the pH/Temperature sensitive thermal gelation of Polypeptide Aqueous Solution.

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Luminescent Lanthanide-Dendrimer Complexes Based on Benzoquinoxaline Derivatives for Optical Amplifications

엄유경, 유정호, *오정환, **송복주, ***PRAMOD, ***이광섭, 김환규, ****Jean-Claude G. Bünzli

*고려대 신소재화학과 *고려대 소재화학과 **고려대(세종) 신소재화학과 ***한남대 신소재공학과 ****École Polytechnique Fédérale de Lausanne (EPFL)*

We have systematically designed and developed novel lanthanide-cored supramolecular systems with highly efficient light-harvesting dendritic arrays for advanced information technology. The benzoquinoxaline based on dendrimeric ligands have been designed and synthesized in order to provide enough coordination sites for the formation of stable Er(III)-chelated complexes. Lanthanide ions were effectively encapsulated by benzoquinoxaline ligands. To obtain the high fluorescent quantum yields and the efficient light-harvesting effect through dendritic chromophores to lanthanide ions, benzoquinoxaline dendrons have been used as photon antenna for the lanthanide-cored supramolecular systems.

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Stereochemical Effect of Polypeptide Based Polymeric Thermogel on Chondrocytes 3D-Culture

최보규, *박민희, **윤은정, 정병문

*이화여대 화학나노과학과 *이화여대 나노과학부 **이화여대 바이오융합과학과*

The secondary structures of polyalanine-poloxamer-polyalanine (PA-PLX-PA) hydrogels were regulated by varying L-Ala/DL-Ala ratio of PA. The secondary structural difference led to a difference in the nanostructures of PA-PLX-PA thermogels which were used as a three-dimensional (3D) culture platform for chondrocytes. The β-sheet dominant hydrogel with an appropriate nanofiber population showed an excellent cell proliferation, cell viability, synthesis of sulfated GAG (sGAG), and expression of type II collagen. The research suggests that control of nanostructure of the 3D environment of a hydrogel as a culture medium plays an important role in the redifferentiation of chondrocytes into articular cartilages.

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Fabrication of Nanohydrogels via Hydrogen Bonding-mediated Physical Gelation of Synthetic Hydroxyl-rich Polyamides

정근수, *김세훈, 박종래

*서울대 재료공학부 *KIST 의과학연구센터*

The advent of new controlled release systems has been demanded over the past decade to overcome the instability of therapeutic agents in physiological condition. Hydrogels, often formed by chemical reactions, have been recognized as a promising delivery carrier to improve the bioavailability of drugs by offering various advantages such as acceptable biocompatibility and less toxicity. Here we report a novel hydrogen bonding-mediated physical hydrogeling system. Galactaric acid, a natural monosaccharide diacid containing four hydroxyl groups, was polymerized with oligo-ethylene oxide diamines, to produce hydroxyl-rich polyamides capable of interchain hydrogen bonding. The polymeric hydrogen bonding behaviors in aqueous milieu were examined by changing the repeating unit of diamine monomer. Further, chromophoric monomers were covalently inserted into the polymeric backbone to observe the sol-gel transition and gel stability by fluorescence probing. Nano-sized hydrogelation was then studied for widening the application area of hydrogels.

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UV-curable Polyurethane for Durable Aroma Finishing with Nanocapsules

김태경, *김진수, **박희문

*한국화학연구원 그린화학연구단 환경자원센터 *한국화학연구원 화학소재연구단 정보전자폴리머연구센터 **한국화학연구원 신화학연구단*

Recently, the biggest challenge of the textile's finishing is fragrance durability, which includes two aspects: scent releasing lifetime and aroma wash fastness. With encapsulated technology, aroma capsules can generate scent for long periods. However, the capsules don't have affinity for textiles.For durable aroma finishing, in which a fabric is cured at 130-170℃ for minutes to make crosslinking. During curing, nevertheless, the aroma inside capsules can escape or be lost through quick evaporation and swelling or break the capsule. The loss from capsules can seriously reduce the aroma amount on the fabric and decrese the durability. To avoid the thermal process, a UV curing resin can be used to fix capsules because the resin can be cured under UV light at low temperatures in seconds. Also UV-curable coating is one of environment-friendly finishing methods for textile because this technology not only overcomes the problem of the high VOC-emission but it also reduces the energy consumption. In this study, we selected the polyurethane acrylate(PUA) resin and the optimal condition for printing with aroma nanocapsule. The PUA resin was synthesized by prepolymg. polypropylene glycol(PPG)/polyethylene glycol(PEG) mixed polyether diol and 4,4,-diphenylmethane diisocyanate (MDI) and then reacting with hydroxyethyl(meth)acrylates. The synthetic PUA resin exhibited high adhesive properties, superior wash fastness for cotton.

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Development of High contrast bimodal imaging probe for Coherent Anti-Stokes Raman scattering (CARS) microscopy

김주환, *정상전

*과학기술연합대학원대 나노바이오공학과 *한국생명공학연구원 바이오나노연구단*

CARS detects chemical bond vibration, thereby visualizing lipid molecules even in the cells without a specific labeling such as fluorescence or radioisotope. Cell penetration mechanism of nanoparticles (NP) is of a major interest in the area of nanobiology. Although cell penetration of polystyrene nanoparticle (PSNP) was measured using CARS, the clarity of the signal was prohibited by lipid droplets in cells. Since the signal interference came from similar vibration energies of aliphatic C-H and aromatic C-H bonds, dueterio-PSNP (DPSNP) have designed and prepared as a high contrast CARS probe as well as a novel tool to study a mechanism of celluar penetration of NP. In addition, DPSNP was labelled with fluorescence to conform the measured CARS signal by fluorescence measurement at the same time. When applied and measured in cells, DPSNP showed a strong CARS signal at the specific wavelength (857 nm) corresponding to C-D bond vibration. Fluorescence measurement conformed that the CARS signal came from DPSNP. DPSNP image was not interfered by aliphatic C-H bond vibration from lipid droplets in the cells thereby showing clear DPSNP images in the cells.

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Silica Nanocontainer using sugar responsive boronic acid and cyclodextrin Gatekeepers for controlled release of guests

이진우, 김세희, 김철희

인하대 고분자공학과

본 연구에서는 MCM-41 타입의 실리카 나노입자 (SiNP, 직경 60 nm, pore 2 nm)의 pore 입구에 gatekeeper 를 장착하고, sugar 와 binding affinity 가 좋은 boronic acid 를 도입하여 sugar 에 의해 pore 내부에 봉입된 guest 분자를 방출시킬 수 있는 나노 전달체를 설계, 제조하였다. 본 연구의 SiNP 시스템에서 gatekeeper 역할을 하는 cyclodextrin (CD)으로 인해 Guest 분자는 pH 8.0 이상의 조건에서 장시간 동안 pore 안에 encapsulation 될 수 있다. pH 가 9.8 에서 guest 분자가 pore 밖으로의 방출이 억제 된다. 또한 pH 7.4 의 조건이나 boronic acid 와 CD 의 결합력 보다 더 강한 결합력을 가진 D-fructose, D-galactose 등을 첨가하면 gatekeeper 로 도입된 CD 가 교환되어서 pore 에 있던 guest 분자가 방출될 수 있도록 설계되었다. 이렇게 설계된 나노 전달체의 크기 및 구조, guest 분자의 로딩 및 방출 정도를 FT-IR, TEM, SEM, fluorescence spectrum, zeta-potential 등으로 확인하였다. 본 연구에서 고안된 시스템은 나노 전달체로서 이용성이 클 것으로 기대된다.

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Imaging and Drug Delivery Systems Using GSH-Rsponsive Nanocontainers Capped with Cyclodextrin.

김세희, 이진우, 김철희

인하대 고분자공학과

본 연구에서는 iron oxide(직경 15nm)를 가지는 MCM-41 타입의 실리카 나노입자 (Fe@SiNP, 직경 60nm, pore 2nm)의 pore 입구에 분자밸브를 창착하여, pore 내부에 봉입된 약물을 특정한 외부 자극을 가하여 방출시킬 수 있는 새로운 방법을 확립하였다. Fe@SiNP 의 표면에 외부자극에 반응할 수 있는 다이설파이드 결합, gatekeeper 로 cyclodextrin (CD)이 도입되었다. 본 시스템에서는 glutathione (GSH)이 없는 조건에서 약물이 장시간 동안 pore 밖으로의 방출이 억제되며, GSH 이 있는 조건에서는 다이설파이드 결합이 분해되어 CD 가 제거되면서 약물을 조절 방출시킬 수 있다. Fe@SiNP 의 구조와 특성은 FT-IR, BET, TEM, SEM, fluorescence spectrum 등으로 규명하였다. 본 연구의 결과는 자기공명영상을 위한 대표적인 iron oxide 로 인해 진단도 가능할 뿐만 아니라 치료까지 가능한 나노 전달체로의 이용성이 클 것으로 기대된다.

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새로운 triazine building block를 이용한 helix와 nanotube의 제조

고윤수, 이정훈, 이진우, 김철희

인하대 고분자공학과

낮은 분자량을 갖는 자기조립형 물질은 규칙적인 배열을 갖는 나노튜브와 helix 구조를 형성한다. 본 연구는 헤테로고리인 1,3,5-s-triazine 분자를 기초로 하여 젤을 형성하는 물질로 잘 알려진 cholesterol 을 결합한 새로운 자기조립형 물질을 설계, 합성 하였다. 이 연구에서 사용된 cyanuric chloride 는 세 개의 염소 원자가 다양한 친핵체에 의해서 선택적인 반응성을 가지므로 여러 가지 ABC 형태의 물질을 합성할 수 있다. 1,3,5-s-triazine 분자를 기초로 하는 gel 시스템의 장점은 도입하는 친핵체의 종류에 따라서 선택적으로 젤을 형성하는 것이 가능하고, 금속이온 센서, 무기 템플레이트 등 여러 분야의 핵심 물질로 응용이 가능하다. 새로운 분자 구조의 triazine 덴드론 유기젤은 자기조립 현상에 의해 helix 및 나노튜브의 구조를 가지므로 다양한 방법을 통한 구조분석을 수행하였다.

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Self-Assembled Dendron-Cyclodextrin Nanotubes with Surface tripeptides and their Biosensory Characteristics

이정훈, *Lohani Chuda Raj, *이건형, 김철희

*인하대 고분자공학과 *인하대 화학과*

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 위의 나노튜브를 metal ion sensing 에 응용하기 위하여 copper ion 과 specific binding 할 수 있다고 잘 알려진 peptide sequence 인 Histidine-Glycine-Glycine 을 CD 의 C6 위치에 형성하였다. 또한 peptide sequence 끝에 fluorophore 로 dansyl derivative 를 도입하였다. 이를 이용하여 표면이 oligo peptide 로 덮인 나노튜브로 self-assembly 되게 하였고, SEM, TEM 등으로 확인하였다. 또한 copper ion 이 binding 한 경우 fluorophore 의 fluorescence 가 quenching 되는 것을 이용해 copper ion sensing 이 가능한 나노튜브센서를 고안하였다

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Anisotropic Proton Conduction of Block Copolymer Electrolyte Membranes Containing Ionic Liquid

김성연, *박문정

*포항공과대 첨단재료과학부 *포항공과대 화학과*

Proton exchange membrane fuel cells (PEMFC) offer the prospect of supplying clean electrical power for a wide variety of systems such as portable electronic devices and vehicles. Significant effort has been devoted to improvement of the transport properties of PEMs which is operated relatively lower temperature below 80 oC. In these days, since the operation at lower temperature than 100℃ makes a problem such as CO poisoning at Pt catalysis, complexity of water and heat management system, great attention has been paid to the development of polymer electrolyte membranes which can conduct proton above 100℃ without humidification. In this study, various SnMBm block copolymers / ionic liquid membranes are prepared to be aimed for elevated PEMFC operating temperature (above 120 oC). In this case, ionic liquid acts as proton supplier under the anhydrous condition and our system is proved to be thermally & mechanically stable up to 180 oC. The increase in sulfonation level of SnMBm copolymers and/or ionic liquid loadings brings overall increase in proton conductivity and the maximum conductivity of 0.045 S/cm is obtained with S50MB73(66) containing 50wt% of 1,3-dimethylimidazolium methane sulfate in anhydrous condition. It is worthwhile to note that the conductivity obtained in our synthetic SMB copolymer system is 40 times higher than that of commercial Nafion.

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Absorption of Sulfur Dioxide in Task-Specific Ionic Liquids

홍성윤, 김대원, 김진형, 정민석, 김훈식

경희대 화학과

New experimental results are presented for the solubility of sulfur dioxide in ionic liquids at 323K and 0.67 atm. [MeSO3] as the anion and imidazolium cations with various pendant groups were used to investigate cation effects on SO2 absorption and desorption.

대한화학회 THE KOREAN CHEMICAL SOCIETY

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Highly efficient metal-free membranes for the separation of acetylene/olefin mixtures: Pyrrolidinium-based ionic liquids as acetylene transport carriers

정스런, 정민석, 김훈식

경희대 화학과

Pyrrolidinium-based ionic liquids with a basic anion were shown to be highly effective acetylene transport carriers for the selective separation of acetylene in ethylene through membranes. The selectivity of acetylene over ethylene varied significantly depending on the type of the anion of the pyrrolidinium-based ionic liquids. The highest selectivity of 23 was attained when 1,3-dimethylpyrrolidinium methylphosphite ([DMPyrr][MeHPO3]) was used as the transport carrier. Computational calculation and 1H NMR results on the interactions of acetylene and ethylene with [DMPyrr][MeHPO3] clearly indicate that the higher selectivity of acetylene over ethane is originated from the specific acid-base interaction between methylphosphite anion, [MeHPO3]- and the acidic hydrogen atom(s) of acetylene.

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Electro-catalytic Performance of PtRu Nanoparticles Deposited on PPy-GNFs for Methanol Oxidation

박정민, 박수진

인하대 화학과

In this work, the polymer composites prepared with polypyrrole (PPy) and graphite nanofibers (GNFs) [PPy-GNFs] were synthesized by in situ polymerization of pyrrole on GNFs. The addition of GNFs to PPy imparted a high activity, which might be due to higher electrochemically accessible surface area and electronic conductivity. So, PPy-GNFs were introduced as PtRu catalyst supports via chemical reduction method. The surface and structural properties of the PPy-GNFs were characterized by Fourier transform spectroscopy (FT-IR) and X-ray diffraction (XRD). The morphological structures of the PtRu/PPy-GNFs catalysts were analyzed by transmission electron microscopy (TEM) and scanning electron microsopy (SEM). The electrocatalytic activity of the catalysts was investigated by cyclic voltammetry measurement. As a result, PtRu nanoparticles were found homogeneously dispersed in PPy-GNFs composites ascertained from SEM and TEM. And, the catalytic performance of PtRu/GNSs was exhibited better electrocatalytic activity than derivative of GNFs for methanol oxidation. Consequently, it was found that PPy-GNFs as catalyst supports could influence on the characterization of the catalysts, indicating PPy-GNFs might have potential application as catalyst supports for fuel cells.

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Effect of KOH Activation on Carbon Supports for PtRu catalysts of Direct Methanol Fuel Cells

박정민, 박수진

인하대 화학과

In this work, multi-walled carbon nanotubes (MWNTs) and carbon blacks (CBs) used as carbon supports were modified by KOH activation in order to improve their properties. The PtRu deposited on CBs/MWNTs were prepared by impregnation method and characterized by BET, X-ray diffraction (XRD), and transmission electron microscopy (TEM). Electrochemical behaviors of the catalysts for methanol oxidation were investigated by cyclic voltammetry (CV). As a result, it was found that KOH activation could influence on the properties of CBs/MWNTs, indicating that the size and loading content of PtRu deposited on the modified carbon supports could be changed. In addition, electro-catalytic activity of the catalysts was enhanced with changed properties of the carbon supports. Consequently, it was considered that the properties of the carbon supports could significantly affect the methanol oxidation of anodic electrocatalysts in DMFCs.

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Silicon Based Inorganic/Organic Hybrid Materials for Highly Efficient Deep Blue Phosphorescent OLEDs

위경량, 강상욱

고려대 소재화학과

Efficient deep blue phosphorescent OLED was achieved in the simple device structure of ITO/ SiTPA/SiCBP : FIr6 10 wt% / SiTAZ / Liq / Al, where active layers were silicon based inorganic/organic hybrid materials of the types, SiTPA, SiCBP, and SiTAZ for HTL, EML host, and ETL respectively. Silicon incorporation into organic framework not only provided necessary morphological stability, but also engaged enhanced charge transporting capability and high triplet energy state essential to achieve highly efficient deep blue PHOLEDs. As a result, high performance silicon based HTL, EML host, and ETL materials were developed, exhibiting high charge mobility values in the range of 10-4 ~ 10-3 cm2V-1s-1 and high triplet energies of 2.84 eV, 3.05 eV, and 2.88 eV, respectively. Even with the simple three layer device structure of PHOLEDs comprising silicon based active layers, maximum external quantum efficiency (EQE) of 19.8 % and CIE coordinates of (0.15, 0.22) were achieved. Moreover, an EQE of 17.5% was recorded at a luminance of 1000 cd m-1, which was the result of reduced efficiency roll-off due to the efficient confinement of FIr6 triplet energy by surrounding silicon based inorganic/organic hybrid materials developed in this work.

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Highly Efficient Electron-Transport Materials based on Bis(4-(4,5-diphenyl-4H-1,2,4-triazol-3-yl)phenyl)dimethylsilane for Deep Blue Phosphorescent OLEDs

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. In consequence, development of new wide band gap 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 are still required for efficient deep blue PHOLED. In this study, to obtain wide energy gap ETL materials with high thermal stability and high electron mobility, silicone atom was introduced between two 3,4,5-triphenyl-1,2,4-triazole molecules by direct substitution reaction between 2 equiv of 3-(4-lithiumphenyl)-4,5-diphenyl-1,2,4-triazole (LiTAZ) and dichlorodimethylsilane. The final product of bis(4-(4,5-diphenyl-4H-1,2,4-triazol-3-yl)phenyl)dimethylsilane (SiTAZ) was exhibited high triplet energy of 2.84eV, high Tg of 115°C and high electron mobility of 1 x 10-4cm2 V-1 s-1. High external quantum efficiency (16.2 %), reduced efficiency roll-off at high luminance (14.5 % at 1000 Cd m-2), and deep blue color coordination (0.16, 0.23) were achieved for Fir6-based PHOLED by using the SiTAZ as an ETL material.

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1,1-Bis(4-(N,N-di-p-tolylamino)phenyl)silane as Hole-Transport Materials for Highly Efficient Deep Blue Phosphorescent OLEDs

김주은, 위경량, 강상욱

고려대 소재화학과

Three 1,1-bis(4-(N,N-di-p-tolylamino)phenyl)silane with non-cyclized dimethylsilane (2-Me) and cyclized 1,1-silacyclopentane (2-Cy5) or 1,1-silacyclohexane (2-Cy6) were prepared from direct substitution reaction between 2 equiv of 4-(N,N-di-p-tolylamino)phenyllithium (1) and corresponding dichlorosilane precursors. All three compounds were characterized by X-ray structural studies and 1H and 13C NMR spectra. In accordance with such an increase in the molecular rigidity, 2-Cy5 and 2-Cy6 exhibited much higher Tg values (78 ºC and 80 ºC, respectively) than the acyclic analogue, 2-Me, while all compounds were unperturbed triplet energy (2.8 eV). By employing 2-Cy6 as a hole-transporting 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 17.8%, an EQE of 16.1% at high luminance of 1000 cd m-2, and deep blue color coordinates of (0.16, 0.22) were achieved.

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New Concepts for Highly Efficient Phosphorescent OLEDs.

황아름, *조대원, **강상욱

*고려대 신소재화학과 *고려대 광전자신소재연구소 **고려대 소재화학과*

As for the Ir(III) based complexes, tuning of emission colors over entire visible spectra has been achieved by modification of both heterocyclic cyclometalates and/or third chelating anions that are generally represented by C^N and L^X, respectively. Usually, the triplet state of the ancillary ligand lies well above the energies of the C^N ligand and MLCT excited states. Therefore, the luminescence is dominated by C^N and MLCT transitions, leading to efficient phosphorescence. If the triplet-state of the L^X ligand is lower in energy than the C^N 3(π-π*) or 3MLCT, metal complexes have their excited states localized predominantly on the L^X ligand and leading to weak phosphorescence from C^N 3(π-π*) or 3MLCT because of the energy sinking from C^N ligand to non-luminescent L^X ligand. Most possible mechanism was proposed as exothermic interligand energy transfer (ILET) from the C^N ligand to the L^X ligand.In this work, our interesting for heteroleptic Ir complexes is the ILET from the C^N ligand to the luminescent L^X ligand. We have been investigated the photophysical properties for ILET in newly synthesized Ir complexes [(dfppy)2Ir(dpq)] and [(dfppy)2Ir(tpphz)], where dpq is 2,3-bis(2-pyridyl)-qinoxaline, dfppy is 2-(4,6-difluoro-phenyl) pyridine) and tpphz is tetrapyrido[3,2-a:2`,3`-c:3``,2``-h:2```,3```-j]phenazine, which have two different emitting C^N (dfppy) and L^X ligands (dpq or tpphz).

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Adsorption of CO_2 onto Amine-grafted SBA-15 Equilateral Hexagonal Platelet

맹룡월, 박수진

인하대 화학과

The characteristics and CO_2 adsorption of SBA-15 equilateral hexagonal platelets (SBA-15-EHP) with 300 nm of thickness and 1.5 μm in diagonal length, modified by mono- and di-aminosilanes were examined in this study. The microstructure of amine-grafted SBA-15-EHP was characterized by XRD and N_2 adsorption, and the content of nitrogen was confirmed by XPS. The CO_2 adsorption behaviors were evaluated by PCT (pressure-composition-temperature) apparatus at 273 K and 1.0 atm. It was found that the presence of nitrogen led to an increase in the CO_2 adsorption capacity of the SBA-15-EHP. The adsorption data showed that SBA-15-EHP possessing a proper pore size exhibited the best CO_2 adsorption capacity as 53.0 mg CO_2/g at 273 K. The adsorption of grafted amine under anhydrous CO_2 could be considered to proceed through carbamate intermediate and zwitterion mechanism.

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Synthesis of Carbon Nanofibers on Fe, Ni, Co/Carbon Fiber Surfaces

맹룡월, 박수진

인하대 화학과

In this work, pyrolytic decomposition of C2H2 on the surface of nickel-, cobalt-, and iron-containing carbon fibers (CFs) has been studied. We found that the high density CNFs were prepared by decomposition of C_2H_2 on metal-doped mesoporous silica films coated CF surfaces at 973 K. It was dependent on the metal catalysts are highly dispersed into molecularly well-defined mesoporous silica structures by complexes of a surfactant with metal cations. This method was more effective than other methods such as controlling the diameter of the carbon materials, enhancing the contact of the carbon nanomaterials to the CF surfaces, and eliminating the requirement of purity of catalysts. SEM and TEM results indicated that the grown CNFs with a diameter between 20 and 100 nm were grown uniformly and densely on carbon fiber surfaces, and the grown CNFs had a herringbone structure.

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Development of liquid fuel formulations by Alkylammonia borane for hydrogen fuel cell: Highly Concentrated Ammoniaborane Solution

김태영, 강상욱

고려대 소재화학과

Alkyl ammonia-borane (AAB) compounds were synthesized and used as hydrogen storage materials. RnNH3-nBH3 (n=1; R= Me, Et, iPr, Ph, n=2; R= Et) were prepared by addition of BH3•SMe2 to corresponding amines. NH3•BRH2(R= iPr, Ph) was prepared from LiBRH3 and (NH4)2SO4. Hydrogen generation from the AAB compounds was carried out with KH14 catalyst at room temperature. To a stirred tetraglyme solution (0.70 M) containing AB or AAB, 2 mole% of KH14 was added at 25 °C. Most AB and N-alkyl/-aryl ABs discharged two equiv H2 within less than 60 seconds whereas B-alkyl or -aryl ABs released only one equiv H2 at slower kinetics of 90 seconds. Furthurmore, 2 equiv of H2 is rapidly released from highly concentrated (11 M) MeAB solutions at 25°C, providing 3.0 system wt % hydrogen release. To further maximize the gravimetric H2 density, AB-AAB mixtures were evaluated. Initial results using a 1:2 AB/Et2AB mixture at room temperature indicate that 2 eq. H2 release can be achieved with 2 mole% of KH14 under solvent-free conditions.

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폐금속을 이용한 Cr(VI)의 환원

김종현

경북과학대학 화장품계열

크롬은 염료, 가죽산업, 금속산업 등 다양한 산업에 많은 양이 사용되는 필수 무기재료이다. 자연상태에서 가장 안정한 형태는 Cr(III)와 Cr(VI)이며 Cr(III)보다 Cr(VI)이 고독성을 갖고 있으며 그러므로 크롬은 환원반응에 의해 독성이 제거될 수 있는 대표적 오염물질이다. 환원반응은 다양한 환원제를 사용할 수 있으나 반응과정에서 2 차적 오염이 되지 않아야 하고 대량으로 사용될 경우 경제적 경쟁력이 있어야 한다. 철산업에서 대량 발생하는 폐금속은 비교적 저독성이며 가격이 저렴하다. 본 연구에서는 철가공공장에서 수거된 폐철을 이용하여 Cr(VI)의 환원반응을 수행하였다. 폐철은 Cr(VI)을 성공적으로 환원하였으며 반응속도는 매우 빨라 공학적 적용이 가능할 것으로 판단된다. 폐철, 폐강철, 폐알루미늄 등에서 폐철이 가장 좋은 반응성을 보여주며 이는 폐철에서 철성분이 가장 많이 포함되어 있으며 산화가 쉽게 되는 것이 원인이라 생각된다. 기존 연구에서와 같이 폐금속의 표면에 묻어 있는 불순물에 의한 영향이 매우 크며 산세척, 용매세척 등의 방법에 의해 제거가 가능한 것으로 나타났다.

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폐철을 이용한 유독오염물의 환원적 분해

김종현

경북과학대학 화장품계열

오염물질의 독성은 다양한 반응에 의해 완화되거나 제거될 수 있다 그러나 현재 공학에서 사용하는 반응은 대부분 산화반응이며 이는 유기오염물질에 쉽게 적용된다. 환원적 분해반응의 경우 유기물질이 이미 산화되어 있는 경우에 매우 유리하다. 최근 주목받고 있는 연구에 의하면 고독성의 염소계유기물질의 경우 환원적 분해반응에 의해 독성이 비교적 쉽게 제거되는 것으로 나타나고 있다. 다양한 환원제 가운데 영가금속의 환원력이 반응에 이용될 만큼 크며 특히 영가철의 경우 환경에 노출되어도 2 차적 독성이 적으므로 많은 연구가 진행되어왔다. 우리나라는 철강산업이 매우 발달하여 있으며 철강제의 사용이 매우 많다. 그리고 철가공과정에서 발생하는 철부산물은 수거되어 다시 재활용된다. 본 연구에서는 철가공과정에서 발생하는 철부산물을 이용한 대표적 염소계독성물질에 대한 분해반응연구를 수행하였으며 trichloroethylene, tetrachloroethylene 등의 산업독성물질이 환원분해반응에 의해 제거되는 것을 확인할 수 있었다. 반응성에 가장영향을 미치는 인자는 철부산물표면의 불순물이며 대량이용에 가장 중요한 장애물은 철부산물표면에서 기름 등의 불순물을 효율적으로 제거하는 것이라 판단된다.

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난연성 세정용제 개발 연구

이윤아, 유영, 김석찬

국민대 화학과

MC, acetone 등의 유기 용제를 사용한 세정법은 좋은 세정력을 가지고 있다. 하지만 이 같은 유기용제는 낮은 인화점으로 인하여 세정 시 화재의 위험과 인체의 해로움 등의 여러가지 문제점을 가지고 있다. 그래서 난연성 세정제 합성을 위해 fluorine 을 도입한 세정제 개발을 연구한다.

한국화학회 THE KOREAN CHEMICAL SOCIETY

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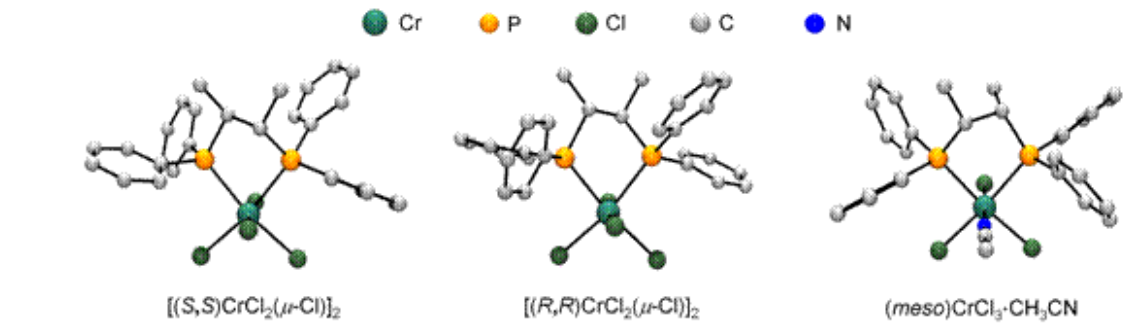
Ethylene Tetramerization Catalysts Based on Cr(III)/DPPDME: Syntheses and Structural Characterizations of [(DPPDME)CrCl3]2 (DPPDME = S,S- and R,R-chiraphos and Meso-achiraphos) Precursors and Optimization of Their Catalytic Performance by Modification of Phenyl Substituents on Phosphines.

정재호, 강상욱

고려대 소재화학과

Cr(III) complexes with chiraphos of S,S- and R,R-stereoisomer and achiraphos of a meso-stereoisomer based on the bis(diphenylphosphino-1,2-dimethyl-ethane) (DPPDME) ligand framework were prepared and characterized structurally to show that the phenyl groups on the phosphine groups determined their catalytic performance for ethylene tetramerization. In particular, chiraphos showed higher catalytic activity, reaching catalytic activities ranging from 1,790~1,929 Kg/gCr/h. Further methyl substitution at the para-position of the phenyl group on S,S-chiraphos, [CrCl2(μ-Cl){(P,P)-κ2-(S,S-DPPDMEp-Me2)}]2 (6), led to unprecedented catalytic performance, reaching a 1-octene activity and selectivity of 2,256 Kg/gCr/h at 45 °C and 77.4% at 25 °C, respectively.



P-Cr-P (°)	79.45	79.90	82.06

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Silicotitanate와 다른 흡착제와 공존할 경우 흡착능력 변화

전종원, *김영훈, **김종현, *강채훈

*안동대 응용화학과 *안동대 환경공학과 **경북과학대학 화장품계열*

현재 미국을 비롯한 선진국에서는 방사선 물질을 제거하기 위해 실리코 티타늄 산화물과 다공질 흡착제를 이용한 연구가 진행되고 있으며 보다 좋은 흡착 능력과 선택성을 얻기 위해 다양한 합성방법과 후처리 연구가 진행 되고 있다. 방사선 핵 종 물질인 Cs, Sr 에 대한 흡착능력의 향상과 선택적인 흡착능력을 얻기 위하여 silicotitanate 와 다른 무기물 흡착제를 이용하여 연구를 수행하였다. 실험에 앞서 사용 할 silicotitanate 는 본 실험실에서 합성한 것으로 단일 성분인 Cs, Sr 에 대해서 선택성과 흡착능력이 좋은 것으로 나타났다. Silicotitanate 의 경우 결정 구조를 가지고 있어 core 안에 Na+ 와 이온교환에 의해서 양이온을 침입시키는 방법이다. Zeolite 는 미세한 결정자 내부 또는 판상 결정자 사이에 양이온이 들어가는 메카니즘을 통하여 흡착이되며 본 연구의 주요시도는 이들 두 흡착제가 공존할 경우 흡착 경향에 관한 것이다. 연구결과 예상과 달리 각 흡착제의 흡착 능력이 감소 하였다. hydroxyapatite 과 혼합한 경우도 흡착능력이 감소하였다. 이는 서로 다른 무기물 흡착제가 공존하면서 흡착제 간의 상호 작용 또는 상호간 이온교환에 의하여 양이온의 이온교환능력과 흡착능력이 저하 하는 것으로 사료된다.

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Significance of Hydrophilic Characters of Organic Dyes in Visible-Light Hydrogen Generation Based on TiO2

전지송, 강상욱

고려대 소재화학과

Considerable attention has been paid to semiconductor TiO2 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 TiO2, dye modification has been used to make TiO2 active to visible-light excitation, typically in dye-sensitized H2 generation using platinized TiO2 particles (Pt/TiO2). In this study, a series of dyes was synthesized to examine the roles of the hydrophilic characteristics of methoxymethyl group in sensitized hydrogen generation by dye-grafted Pt/TiO2 under visible light irradiation. The hydrogen-generation efficiencies and optimum amounts of the dyes grafted to Pt/TiO2 were affected substantially by the hydrophilic and steric effects of methoxymethyl group. Moderately hydrophilic compounds showed higher sensitization activity at a lower loading than hydrophobic compounds.

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Sterically Less Hindered Half-Titanocene(IV) Phenoxides: Ancillary Ligand Effect on Mono-, Bis-, and Tris-(2-Alkyl/Aryl-Phenoxy) Titanium(IV) Chlorides

김태진, 강상욱

고려대 소재화학과

A series of mono-, bis-, and tris-phenoxy titanium(IV) chlorides of the type Cp*Ti(2-R-PhO)nCl3-n (n = 1, 2, 3) was prepared, where R = Me, iPr, tBu, and Ph groups. The formation of each mono-, bis- and tris-2-alkyl/aryl phenoxy series was authenticated by structural studies on representative examples of the phenyl series including Cp*Ti(2-Ph-PhO)Cl2 (1PhCl2), Cp*Ti(2-Ph-PhO)2Cl (2PhCl), and Cp*Ti(2-Ph-PhO)3 (3Ph). The metal coordination geometry of each compound is best described as pseudo-tetrahedral with the Cp* ring and 2-Ph-PhO and chloride ligands occupying three leg positions in a piano-stool geometry. The mean Ti–O distances observed with increasing number of 2-Ph-PhO groups, showing values of 1.784(3), 1.802(4), and 1.799(3) Å for 1PhCl2, 2PhCl, and 3Ph, respectively. All four alkyl/aryl series with Me, iPr, tBu and Ph substituents were tested for ethylene homo-polymerization after activation with Ph3C+[B(C6F5)4]- and mMAO-7 at 140 °C. The phenyl series showed much higher catalytic activity ranging from 43.2 and 65.4 Kg/(mmol of Ti•h) than the Me, iPr, and tBu series (19.2 and 36.6 Kg/(mmol of Ti•h)]). Among the phenyl series, bis-phenoxide of 2PhCl showed the highest activity of 65.4 Kg/(mmol of Ti•h). Therefore, the catalyst precursors of the phenyl series were examined by reacting them with a variety of alkylating reagents, such as, trimethylaluminum (TMA), triisobutylaluminum (TIBA), and methylalumoxane (MAO). In all cases, 2PhCl produced the most catalytically active alkylated species, Cp*Ti(2-Ph-PhO)MeCl. This was further supported by DFT calculations based on the simplified model with TMA.

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Generation of Ru Heteroleptic Complexes by Band-Gap Control of the Bipyridyl Ligand System: Synthesis, Characterization, and Dye-Sensitized Solar Cells (DSSCs) Application.

한중규, *조대원, **강상욱

*고려대 신소재화학과 *고려대 광전자신소재연구소 **고려대 소재화학과*

Band-gap tunable ruthenium polypyridine sensitizers of the type Ru(NCS)2L(N^N-ArX), where the ligand consists of an 2,2'-bipyridine connected at the 4,4'-position by a 4-substituted aryl functional groups with X = NMe2, OMe, H, Cl, F, and CN, were prepared for dye-sensitized solar cells (DSSCs). We performed the systematic study of the luminescence, visible light absorption, electrochemical, and photoredox property of band-gap tuned ruthenium complexes. Indeed, the introduction of electron-withdrawing groups lowered the LUMO level of ruthenium complex with its decreased band-gap while electon-donating groups showed the relatively high LUMO level with increased band-gap. As a result of this modification, a characteristic difference was observed not only on the molecule spectroscopic and electrochemical properties but also on the device performance. Power-conversion efficiency of Ru-CN was higher than that of N3 under the same cell fabrication and measuring procedures.

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Synthesis of 1,3-disubstituted ureas from CO2 and primary amine catalyzed by ionic liquid.

심유나, 김훈식, 정민석

경희대 화학과

Urea derivatives, especially symmetrical 1,3-disubstituted ureas have an important role in variable application and organic synthesis as a carbonyl compound. Among the alternative way of phosgenation of amines, it has been known that urea can be synthesized from amine and CO2. We discovered that ionic liquid, especially [BMIM]Cl behave as a powerful catalyst for the reaction between primary amines and CO2.

THE KOREAN CHEMICAL SOCIETY

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Development of chemical hydrogen materials for hydrogen fuel cell applications: Catalytic dehydrogenation of diamine bisborane

김성관, 김태영, 김태진, 강상욱

고려대 소재화학과

Diamine bisborane compounds 1-8 were synthesized by addition of BH3•SMe2 to corresponding amines. Dehydrogenation of diamine bisborane catalyzed by transition metal homogeneous catalysts was carried out in non-aqueous solution at room temperatures. The introduction of 2 mol% of (POCOP)Ir(H)2 ((POCOP = [η3-1,3-(OPtBu2)2C6H3]) complex to a solution of ethylenediamine in tetraglyme (0.70 M) resulted in a rapid gas evolution. The H2 purity and quantity were checked and determined by means of quadruple mass spectroscopy (QMS) and mass flow meter (MFM), respectively. Volatiles identified were mainly hydrogen and approximately two equiv H2 were measured.

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Metal-free membranes for the separation of acetylene/olefin mixtures: Imidazolium-based ionic liquids as acetylene transport carriers

이진규, 정스런, 정민석, 김훈식

경희대 화학과

Imidazolium-based ionic liquids with a basic anion were shown to be highly effective acetylene transport carriers for the selective separation of acetylene in ethylene through membranes. The selectivity of acetylene over ethylene varied significantly depending on the type of the anion of the imidazolium-based ionic liquids. The highest selectivity of 19 was attained when 1,3-dimethylimidazolium methylphosphite ([DMIM][MeHPO3]) was used as the transport carrier.

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One-Pot Hydrogen Storage System Based on Si-H/Si-OMe Reversible Process: Hydrogen Release via Methanolysis and Regeneration by Hydride Reduction from Stable Liquid Carbosilane

한원식

고려대 소재화학과

A series of cyclic- and linear carbosilanes, 1–5, were prepared and examined as potential reversible hydrogen storage materials via methanolysis and regeneration by a hydride reduction. In methanol, with the aid of a NaOMe catalyst, cyclic carbosilanes with the formula, (CH2SiH2)3 (1) and (CH2SiH2CHSiH3)2 (2), underwent rapid hydrogen release at room temperature showing only small activation energies, 4.37 kJ/mol for compound 1 and extremely low for compound 2. The storage capacities of compounds 1 and 2 reached 3.76 and 4.30 wt.-% H2, respectively, by combining a stoichiometric amount of methanol with 5 mol% NaOMe. LiAlH4 reduction on each methoxysilyl group in the resulting methoxysilyl carbosilanes, (CH2Si(OMe)2)3 (6) and (CH2Si(OMe)2CHSi(OMe)3)2 (7), resulted in a return to the corresponding starting carbosilanes, 1 and 2, in high yield. Likewise, linear carbosilanes, SiH3CH2SiH2CH2SiH3 (3), SiH3CH2CH(SiH3)2 (4), and SiH3CH2CH(SiH3)CH2SiH3 (5) showed similar reversible hydrogen release and regeneration cycles, recording storage capacities of 4.18, 4.41, and 4.26 wt.-% H2, respectively.

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Effect of KOH Ratios on Hydrogen Storage Behaviors of Activated Carbon Nanotubes

이슬이, 박수진

인하대 화학과

In this study, we prepared the activated multi-walled carbon nanotubes (MWNT) processed by chemical activation with KOH/MWNT ratios in a range of 1:1-5:1, in order to investigate the structure changes produced by different defects of MWNT and the effect on their hydrogen storage behaviors. The FT-Raman spectroscopy was used to test the structure destruction of MWNT after activation. The textural properties of the activated MWNT were investigated by N_2/77 K adsorption isotherms by Brunauer-Emmett-Teller (BET) equation and Dubinin–Radushkevich (D-R) method. The hydrogen adsorption capacities of the activated MWNT were investigated by BEL-HP at 77 K and sub-atmospheric pressure. From the results, it was found that the specific surface area and micropore volume of the MWNT after activation were significantly increased due to the defective structure formed by KOH etching. Consequently, the hydrogen storage capacities of the activated MWNT were improved with increasing KOH reagent, indicating that the micropore volume of the activated MWNT played a key role in the hydrogen adsorption at 77 K.

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Influence of Textural Properties on Hydrogen Storage Behaviors of Nanoporous Carbons

이슬이, 박수진

인하대 화학과

In this study, the nanoporous carbon materials were synthesized by replication from organized mesoporous silicas. The carbonization temperature allowed varying the textural properties of the samples. The microstructure of the samples was characterized by X-ray diffraction (XRD) and transmission electron microscopy (TEM) measurements. N_2/77 K adsorption isotherms were analyzed by Brunauer-Emmett-Teller (BET) and Dubinin-Radushkevich (D-R) plot methods to characterize specific surface area, pore volume, and pore size distribution of the samples. The capacity of hydrogen adsorption of the samples was evaluated by BEL-HP at 77 K/1 bar. From the results, it was found that the hydrogen storage capacity correlated well with the micropore volume determined by applying D-R equation on N_2 adsorption isotherms showing the importance of ultramicropores. Consequently, a linear dependence was found between the hydrogen storage capacity and the micropore volume of prepared samples, rather than with BET specific surface area.

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Preparation and Characterization of Porous Si-loaded Carbon Nanofibers

정기호, 박수진

인하대 화학과

In this work, porous Si-loaded nanofibers were fabricated by electrospinning method. Polyacrylonitrile (PAN) was dissolved in dimethylformamide (DMF) for polymer solution and silicon was dispersed in solution with various silicon content ratios. The nanofibers were used to prepare carbon nanofibers, through stabilization and carbonization processes. The properties of the Si-CNFs were characterized by SEM, TGA, and cyclic voltammetry. The experimental results indicated that the silicon particles were homogeneously dispersed within the CNFs, and the nanofibers had an uniform diameter of approximately 2 μm. The electrochemical activity of the CNFs was gradually improved due to the introduction of silicon particles. Consequently, it was found that the introduction of silicon could affect the electrochemical properties of the CNFs, and the Si-CNFs might have potential applications as anode materials for rechargeable lithium-ion batteries.

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Electrochemical Properties of Polystyrene-based Activated Carbon Nanofibers for Supercapacitors

정기호, 박수진

인하대 화학과

In this work, the polystyrene used as a precursor of carbon fibers was prepared with treatment for improvement of low carbon yield of polystyrene. The treated polystyrene solutions in dimethylformamide were electrospun into webs consisting of 1.8 μm fibers. These fiber webs were used to produce activated carbon nanofibers (ACNFs), through stabilization and carbonization-activation processes. The diameter of ACNFs increased and surface became rougher after activation. The experimental results indicated that ACNFs activated at 800°C afforded the highest specific surface area, mainly due to the micropores, and introduced a maximum specific capacitance at low current density. Consequently, the capacitance was strongly dependent on the specific surface area and micro- or mesopore volume of the ACNFs.

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A study about the influences of catalyst and electrolyte area on photoelectrochemical properties for high performed DSCs

이현정

현대하이스코 환경에너지연구팀

Dye-sensitized solar cells (DSCs) based on titanium oxide 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 11.3%, this technology still has challenges and problems for commercialization such as electrolyte leakage, enlargement, durability, etc.In this study about DSCs, two approaches have been carried out. The first part is the effect of catalyst area on energy conversion efficiency of dye cells. The task of the counter electrode is the reduction of the redox electrolyte used as a mediator in regenerating the sensitizer after electron injection. As a catalyst of redox reaction, counter electrode area could affect photoelectrochemical properties of dye cells. Lab scale dye cells were fabricated with different coating area of catalyst with same working electrode area. In the second, the influence of electrolyte area on efficiency of DSCs has been conducted by fabricating dye cells with different injected electrolyte area.The electrochemical properties of DSCs were investigated by a range of electrical methods as well as by Impedance. Energy conversion efficiency were measured by solar simulator under AM 1.5 condition.

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New Approach toward Processible Metal Bearing Polymers: From Metal Organic Frameworks to Metallopolymers

최은영, 이석현, 권오필

아주대 분자과학기술학과

A systematic study of MOFs has been successfully undertaken by incorporating a homologous series of alkyl side chains with various lengths (the number of methylene unit, n = 6~14) to organic linker, in which the length of alkyl side chain could be key factor to lead to either IRMOF or layered structured polymers. Remarkably, the organic linkers with side chains up to 9 carbons form a three-dimensional network solid whereby the side chains reside in the cavity. As n increased from 10 to 14 carbons, the long side chains not only induced a rearrangement of the framework to give self-layered metallo-polymers, but also imparted a crucial property for processing to the generally intractable metal coordination polymers. Additionally, this system shows the drastic solid-to-solid transformation from IRMOF to layered polymer according to the lengths of alkyl side chain (n = 8, 9). This transformation is attributed to the contribution of the self-layering ability of long alkyl side chain and volume stress due to the occupancy of side alkyl chain within pores.

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Synthesis and Characterization of Nickel(II) Complexes of Mono-functionalized Tetraaza Macrocycles

강신걸, 김현자

대구대 화학과

The mono-*N*-cyanomethylated macrocycle 2-cyanomethyl-5,16-dimethyl-2,6,13,17-tetraazatricyclo[16.4.0.$^{1.18}$0$^{7.12}$]docosane (B) has been prepared by the reaction of 3,14-dimethyl-2,6,13,17-tetraazatetracyclo[16.4.1$^{2.6}$.0$^{1.18}$.0$^{7.12}$]tricosane (A) with 2-bromoacetonitrile. The nickel(II) complex $[Ni(B)]^{2+}$ readily undergoes hydrolysis in aqueous solution to yield $[Ni(C)]^{2+}$ bearing one *N*-CH_2CONH_2 pendant arm. The complexes $[Ni(D)]^{2+}$ and $[Ni(E)]^{2+}$ bearing one *N*-$CH_2C(=NH)OCH_3$ or one *N*-$CH_2(=NH)NHCH_2CH_2CH_3$ pendant arm, respectively, has been prepared by the reaction of $[Ni(B)]^{2+}$ with methanol or n-propylamine. The *N*-CH_2CONH_2 pendant arm of $[Ni(C)]^{2+}$ is deprotonated in basic aqueous solution. The *N*-$CH_2C(=NH)OCH_3$ group of $[Ni(E)]^{2+}$ is protonated in acetonitrile containing $HClO_4$, whereas the pendant arm is not protonated in aqueous solution. Synthesis, characterization, and chemical properties of the mono-*N*-cyanomethylated macrocyclic compounds are presented.

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Reaction of Tetraaza Macrocyclic Complexes Bearing *N*-Cyanomethyl Pendant Arms with Phenol or Salicylaldehyde

강신걸, 김현자, *곽지훈

*대구대 화학과 *순천대 화학과*

Various types of functionalized macrocyclic complexes have been prepared by the reaction of *N*-cyanomethyl groups of $[M(L^1)]^{2+}$ (M = Ni(II) or Cu(II); L^1 = 1,8-bis(cyanomethyl)-5,16-dimethyl-2,6,13,17-tetraazatricyclo[16.4.0.$^{1.18}$0$^{7.12}$]docosane) with phenol or salicylaldehyde. The reaction is promoted by the central metal ion and is strongly influenced by the nature of the central metal ion. The chemical properties of the products are also strongly influenced by the nature of the functional groups. Synthesis, structures, and chemical properties of the products are present.

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Metal-induced C-N Bond Cleavage of Structurally Constrained Tetraaza Macropolycycles

강신걸, 권혜민

대구대 화학과

The structurally constrained tetraaza macrotricycle 2,2,4,10,10,12-hexamethyl-1,5,9,13-tetraazatricyclo[11.3.2.2^{5,9}]eicosane (L^1) reacts with $Cu(OAc)_2.H_2O$ to produce the macrobicyclic complex $[CuL^2]^{2+}$ (L^2 = 2,2,4,10,10,12-hexamethyl-1,5,9,13-tetraazabicyclo[11.3.2]octadecane) under mild conditions, showing that the C-N bonds at one of the two N-CH_2CH_2-N linkages of the macrotricycle are readily broken in the presence of the metal salt. The macrobicyclic copper(II) complex is extremely stable in the solid state and in various solvents. Interestingly, L^2 reacts with $Ni(OAc)_2$•$4H_2O$ to yield $[NiL^3]^{2+}$ (L^3 =5,7,7,13,15,15-hexamethyl-1,4,8,12-tetraazacyclopentadecane). This indicates that the C-N bonds of the two N-$CH_2CH_2CH_2$-N linkage of the macrobicycle are readily broken in the presence of the nickel(II) salt.

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Synthesis of Various Macropolycyclic Copper(II) Complexes with a 5-6-6-6 Chelate Ring Sequence

정수경, *김현자, *강신걸

*김포대학 호텔조리학과 *대구대 화학과*

The hexaaza macrotricyclic copper(II) complex $[Cu(A)]^{2+}$ (A = 1,3,6,8,12,16-hexaazatricyclo[14.3.1.1$^{8.12}$]heneicosane) with a 5-6-6-6 chelate ring sequence has been prepared by the metal-directed condensation of formaldehyde with 1,5,9,13-hexaazatridecane, ethylenediamine, and formaldehyde in the presence of the metal ion. Various pentaaza macrobicyclic copper(II) complexes $[M(B)]^{2+}$ (B = 7-alkyl derivatives of 1,5,7,9,13- pentaazabicyclo[11.2.2]heptadecane) with a 5-6-6-6 chelate ring sequence have been also prepared by the metal-directed condensation of formaldehyde with 1,4-Bis(3-aminopropyl)piperazine and appropriate primary alkylamines. The copper(II) complexes are relatively inert against decomposition even in concentrated $HClO_4$ aqueous solution. Synthesis, characterization, and chemical properties of the macropolycyclic copper(II) complexes are presented.

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Structures and Gas Sorption Properties of MOFs Based on Three Types of Pyridyl Carboxylate Ligands

진나래, 전형필

한양대 응용화학과

A series of new metal-organic frameworks with Fe^{3+} and ligands having both pyridyl and carboxylate moieties is reported. These MOFs are 3D networks based on the same type of trinuclear SBU with the general formula $[Fe_3(O)(CO_2)_6]$. Gas sorption studies using N_2, O_2, Ar, CO_2, H_2 and CH_4 reveal significant differences in the amounts adsorbed and selectivity. We will discuss whether and how non-coordinating pyridyl moieties influence the adsorption properties.

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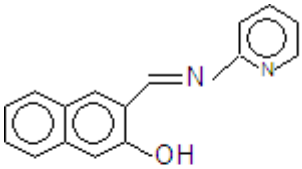
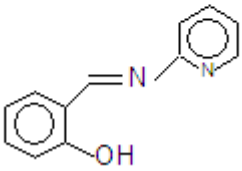
Basic Research of New Dye for Dye Sensitized Solar Cell

김영해, 형은수, 정원목, 전용우

서경대 응용화학과

Basic Research of New Dye for Dye Sensitized Solar CellEun Su Hyeong , Won Mok Jung, Yong Woo Jun and Young Hae KimDepartment of Applied Chemistry, Seokyeong University Until now, the dyes for the dye sensitized solar cells (DSSCs) are being used primarily ruthenium complexes and these dyes are regarded as excellent. Among the ruthenium complexes, the red dye N3 and the black dye N749 are the most prominent. But the price for these materials is fairly expensive, thus developing new dyes are necessary for DSSCs.In this lab, we have investigated the absorption and luminescence spectra of the transition - imine complexes for DSSCs. We have been looking for the imine dye whose maximum absorption wavelength (λmax) is observed at near 510nm (red color) and luminescence intensity is much smaller. Λmax of salicylidene-2-aminopyridine was observed to shift to longer wavelength (blue shift) at higher pH (350nm → 410nm at pH 9). Blue shift for the absorption spectra have not been observed when adding several transition metal ions to salicylidene-2-aminopyridine solution (it is not desirable). But transition metal ions made the luminescence intensity decreased considerably.Compared to salicylidene-2-aminopyridine, 2-hydroxy naphthalidene-2-aminopyridine was observed λmax to be shifted to longer wavelength (350nm → 450nm). The absorption spectra change according to pH change and the effect of several transition metal ions are investigated.Solvent: MeOH + H2O (4:1)Fig.1 Structure of 2-Hydroxy-naphthalidene-2-aminopyridineFig.2 Structure of Salicylidene-2-aminopyridine





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장소: 송도컨벤시아
발표코드: **Ⅰ33P8포**
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발표종류: 포스터, 발표일시: 목 10:30~12:30

Formation of Porous Coordination Polymer Particles Using Blended Building Blocks

이경아, 이희정, 오문현

연세대 화학과

Porous coordination polymers built from metal ions or metal clusters connected by organic building blocks have been extensively studied due to their useful properties and applications such as gas storage, separation, optics, and catalysis. Recently, the several synthetic strategies for the preparation of micro- and nano-sized coordination polymer particles (CPPs) have been demonstrated. The internal structure of CPP is quite important because this dictate the CPP's properties. Herein, we present the formation of porous CPPs with controllable internal structure using blended organic building blocks.

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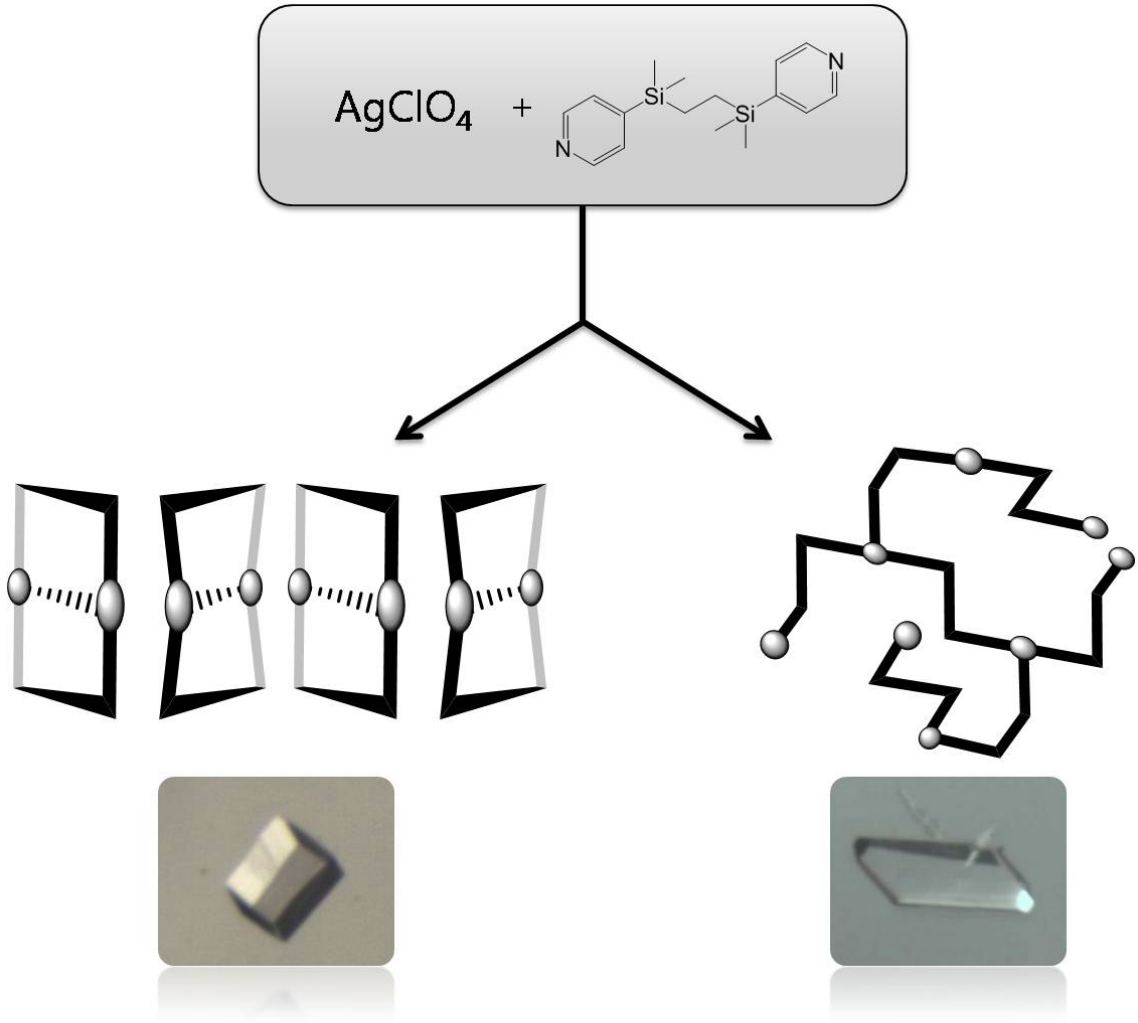
발표종류: 포스터, 발표일시: 목 10:30~12:30

"Metallacyclic Dimer" vs "Interpenetrated 2D Polymer" Induced via the Conformation of Ligand: $[Ag(L)]_2(ClO_4)_2$, $[Ag_3(L)_2]_n(ClO_4)_{3n}$

김치원, 김치원, 정옥상, 정옥상

부산대 화학과

Self-assembly of $AgClO_4$ with 1,2-bis(dimethyl(pyridin-4-yl)silyl)ethane (L) in a mixture of water and acetone affords two shapes of cubic and parallelogram crystals. For the cubic crystal, L connects two silver(I) ions to form two kinds of 26-membered metallacyclic dimers, $[Ag(L)]_2(ClO_4)_2$. The local geometry around the silver(I) ion is a linear arrangement of two Ag-N bonds. Each dimer has slight difference in intracyclic argentophilic interactions (Ag1…Ag1' = 3.346(1); Ag2…Ag2' = 3.243(1) Å), dihedral angles between the two pyridyl rings (19.2(3); 16.6(3) º), and electrostatic interactions (Ag…OClO3 = 2.915(5); 2.797(5) Å). In contrast, parallelogram crystal is consisting of interpenetrated 2-D coordination polymers, $[Ag_3(L)_2]_n(ClO_4)_{3n}$. The local geometry around the silver(I) ion is a trigonal arrangement of three Ag-N bonds. Their compositions and structures are fully confirmed by elemental analyses, TGA, IR, along with X-ray crystallography.


AgClO4 +
Si
Si
N
N

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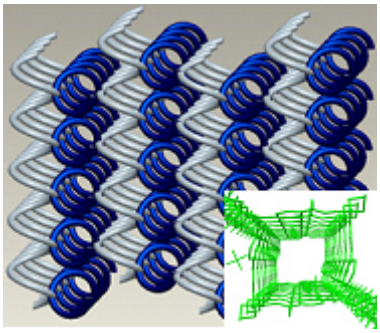
2-Fold Interpenetration via Ligand-induced Alternating Perpendicular Helical Channel Motifs

노태환, 정옥상

부산대 화학과

The reaction of $AgPF_6$ in methanol with 1,3-dibromo-2,2-bis[(isonicotinoyloxy)methyl]propane (L) in dichloromethane affords an acentric diamonoid 3D silver(I) coordination polymer, $[Ag(L)_2]_n(PF_6)_n$, with 2-fold interpenetration with alternating perpendicular "right-handed" and "left-handed" helical channel motifs induced by the bent ligand. The local geometry around silver(I) ion is a tetrahedral arrangement of four Ag-N bonds. The complex could be applied to the development of rational synthetic routes for the ontainment of characteristic topological materials.



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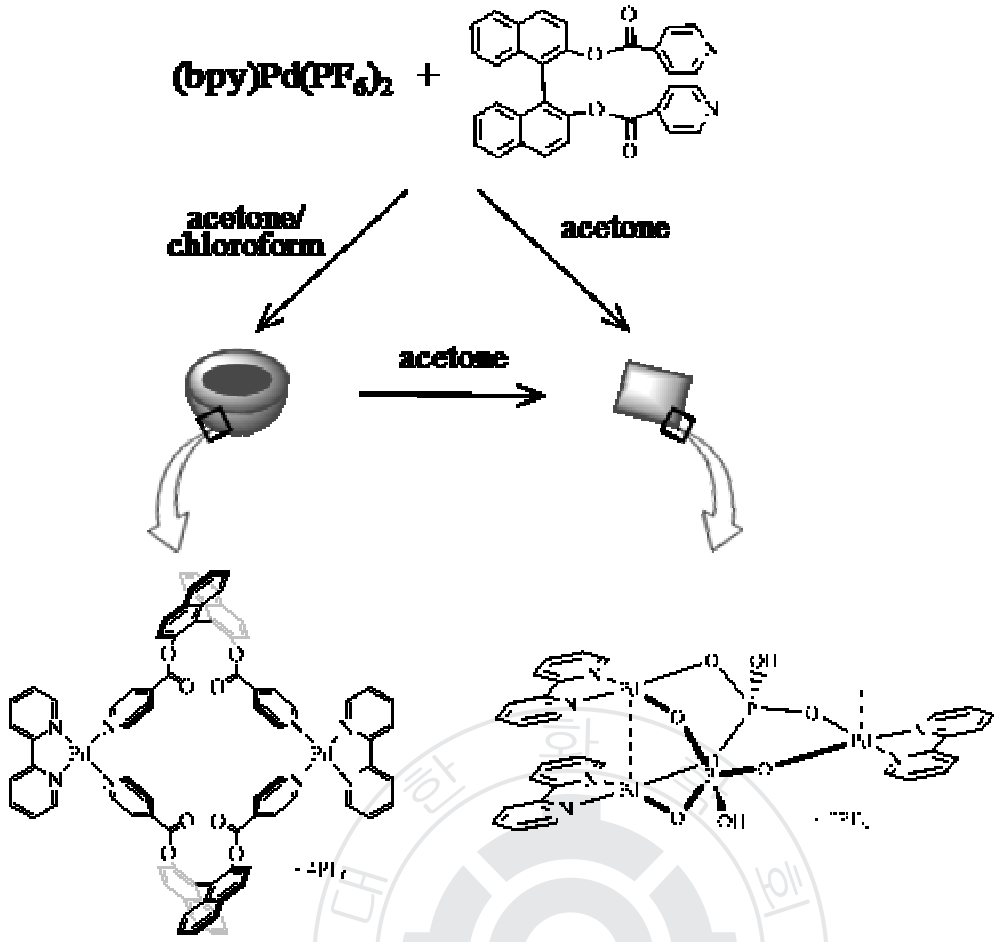
Formation and Related-behavior of Micro-bowl Morphology Consisting of Ionic Palladium(II) Complexes

안정민, 정옥상

부산대 화학과

Reaction of $[(bpy)Pd](PF_6)_2$ (bpy = 2,2'-bipyridine) with racemic bis(isonicotinoyl)-1,1'-bi-2-naphtholate (L) in acetone, and followed by addition of chloroform and solvent evaporation allows to form amorphous micro-bowl morphology consisting of $[(bpy)PdL]_2(PF_6)_4$ without any template or additive. In contrast, the reaction and recrystallization in acetone for 1 week produces parallel-piped single crystals consisting of $[(bpy)_3Pd_3(\mu_3\text{-}HPO_4)_2](PF_6)_2$. The formations of micro-bowl and parallel-piped single crystal morphologies appear to be primarily associated with the kinetic and thermodynamic control, respectively. The formation of micro-bowls may be attributed to eruption of organic solvents. Cosolvent effects and chemical properties on the formation of micro-bowl morphology have been observed.



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Cu(I) Coordination Polymers of 2,4,6-Trithiomorpholino-1,3,5,-triazine

양호진, 박가람, 김태호, 김진은

경상대 화학과

The coinage metal ions such as Cu(I) and Au(I) with the d^{10} electron configuration are known to afford emissive complexes. Simple self-assembly processes involving multidentate ligands and copper(I) halides often lead to coordination polymers with different polynuclear structural motifs. Recently, we have explored coordination polymers based on dithioether ligands and $(CuI)_x$. As an extension of our efforts to investigate Cu(I) coordination polymers of dithioether ligands, we synthesized a tri-sulfur donor lingand, 2,4,6-Trithiomorpholino-1,3,5,-triazine. And, three Cu(I) coordination polymers based on the ligand were prepared. Syntheses, structural characterization, thermal and luminescent properties of these Cu(I) coordination polymers are presented.

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Strong Blue Luminescent Copper(I) Coordination Polymers

김태호, 양호진, 박가람, 김진은

경상대 화학과

Recently, there has been considerable interest in phosphorescent transition metal complexes because of their potential applications in flat-panel displays and lighting sources. We have explored coordination polymers based on dithioether ligands and $(CuI)_x$. 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 $(CuI)_x$ coordination polymers ($x=2,3,\infty$) based on an N/S mixed donor ligand, 4-(3-pyridinylcarbonyl)-thiomorpholine. The results of our investigation including syntheses, structural characterization, thermal and luminescent properties of three new Cu(I) coordination polymers are presented.

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Cu(I) Coordination Polymers of N/S Mixed Donor Ligand

박가람, 양호진, 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, $(CuI)_x$, such as rhomboid dimers, cubanes or stairstep tetramers, 1-D chains, and double-stranded stairs, etc. Recently, we have explored coordination polymers based on dithioether ligands and $(CuI)_x$. 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 and stair-step tetramer Cu(I) coordination polymers based on an N/S mixed donor ligand, $C_{11}H_{16}N_2OS$. The results of our investigation including syntheses, structural characterization, thermal and luminescent properties of two new Cu(I) coordination polymers are presented.

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Synthesis of nanocrystalline TiO_2 by microwave-assisted hydrothermal reaction and the effect of shape of TiO_2 nanoparticle on photovoltaic efficiency.

최민식, 이익모

인하대 화학과

A new synthetic process with easy control of the shape and size of TiO_2. Nanocrystalline TiO_2 was synthesized by microwave-assisted hydrothermal reaction (MH) using titanium isopropoxide(TTIP), and ethanol as starting materials. Tetramethylammonium hydroxide (TMAH) or tetrabuthylammonium hydroxide (TBAH) was used as a surfactant. Each structural shape was selectively controlled by simply changing the concentration of TMAH or TBAH. Various shapes of TiO_2 nanoparticle have been prepared and photovoltaic efficiencies of these materials have been measured. The overall preparative procedure is simple, reproducible, and relatively inexpensive with easy scale-up.

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Convenient synthesis of β-diketimine ligands with dimethylsulfate assisted by microwave.

윤샛별, 이병기, 이익모

인하대 화학과

A novel preparative method of N,N'-β-diketimines with alkyl substituents from 1,3-diketones has been developed. 1,3-Diketone was reacted by alkyl amine in the presence of dimethylsulfate which is known as an O-alkylating reagent. This method can be applied without solvent with easy scale-up and good yield. Dimethylsulfate proves high reproducibility, low cost and potentially safer than conventional agent such as triethyloxonium tetrafluoroborate (Meerwein's salt). Successful synthesis of N,N'-β-diketimines with alkyl substituents will widen further applications in a variety of fields.

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The effects of in-situ ß-ketoiminates and ß-diketiminates on the DCPD polymerization activities of Tungsten catalysts

이응준, 안명용, *성익경, **황운성, 이익모

*인하대 화학과 *코오롱유화(주) 기술연구소 연구1팀 **(주)코오롱 기술연구소*

Dicyclopentadiene (DCPD) has been polymerized by ring opening metathesis polymerization (ROMP) polymerization catalysts based on W & Mo catalysts. The resulting polyDCPD showed some weakness such as presence of gas holes.In order to improve this property, ROMP polymerization of DCPD by tungsten compounds with addition of β-ketoiminates and ß-diketiminates has been carried out and the resulting polymer showed improved hardness and absence of gas holes. The effects of these ligands and several reaction factors on the polymerization activity and polymer properties have been investigated and the results will be presented.

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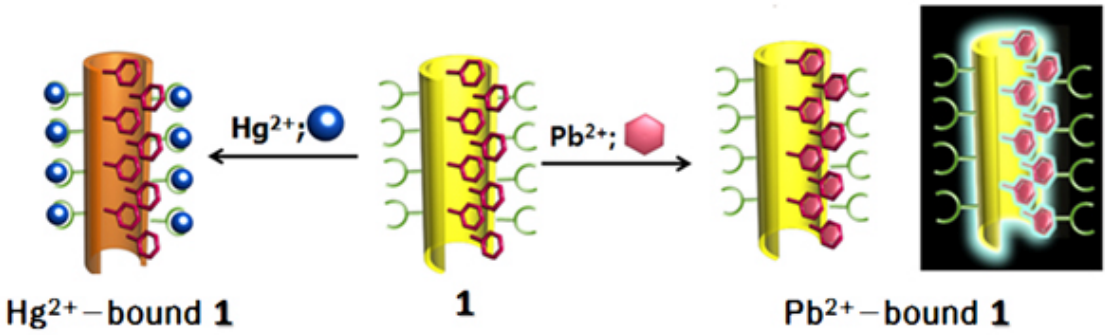
Development of Immobilization Method of Different Functional Ligands onto the Internal and External Surfaces of Silica Nanotubes

서성민, 정종화

경상대 화학과

We synthesized two different chromogenic ligands, which have selectively recognized for Pb^{2+} and Hg^{2+} ions, respectively. Two different-type ligands were attached onto the inner and outer surface of silica nanotubes by sol-gel grafting reaction. We observed the chromogenic and fluorogenic changes of functionalized silica nanotubes upon the addition of metal ions in aqueous solution. The functionalized silica nanotubes selectively recognized for Pb^{2+} and Hg^{2+} ions by each ligands attached onto surface of silica nanotubes.



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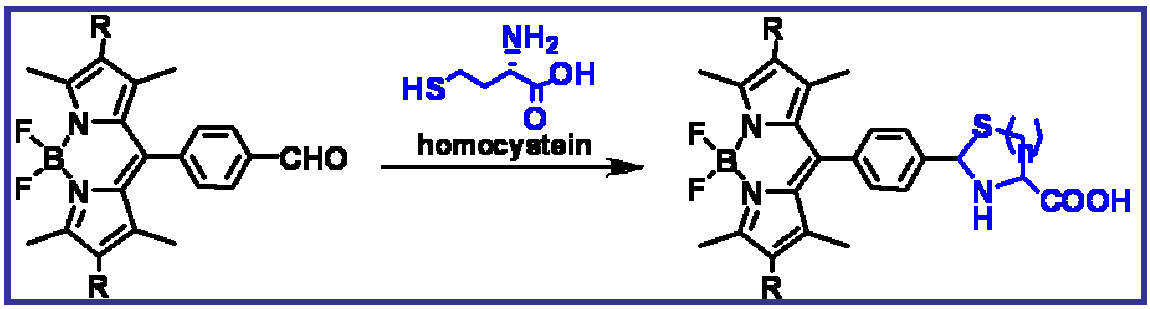
BODIPY Based Derivative for Detection of Homocysteine

손현종, 정종화

경상대 화학과

Homocysteine (Hcy) plays crucial roles in many physiological processes. For instance, an abnormal level of homocysteine is implicated in diseases such as liver damage, skin lesions, slowed growth, and an elevated level of homocysteine is a risk factor for Alzheimer's and cardiovascular diseases. Thus, the detection of homocysteine has been the subject of much attention. Recently, a great effort has gone into the development of selective fluorescence for highly sensitive processes, suitable turn-on fluorescence chemosensors for homocysteine.There fore, The BODIPY derivative was synthesized of the methyl 4-(chlorocarbonyl)benzoate, 2,4-dimethylpyrrole, BF_3-OEt_2, 3-aminophenylboronic acid and 3-(triethoxysilyl) propyl isocyanate. The BODIPY was immobilized onto magnetic slica nanoparticles by sol-gel reaction. In this conference, We Will explain on synthetic method of BODIPY derivative as receptor for homocysteine in detail



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Properties of Porphyrin-Based Coordination Polymer Gel with Pd Ion

조영제, *Jagadese J. Vittal, 정종화

*경상대 화학과 *National University of Singapore, Singapore and Gyeongsang National Uni., Korea*

Tetrakis(4-carboxyphenyl)porphyrin(TCPP) formed gel in the presence of Pd2+ ion without heating process. TCPP polymeric gel was characterized by TEM, FT-IR, UV-Vis spectroscope and Fluorophotometry. The gelation is attributed to the self-aggregation of 1D coordination polymers to form 3D nanostructures through non-covalent interactions to entrap solvent molecules. The freeze-dried polymeric gel exhibits a fibrillar network structure. UV/vis absorption studies illustrate that the TCPP polymeric gel displays a typical π - π^* transition. The fluorescence intensity of the coordination polymeric gel in the presence of Pd^{2+} is quenched dramatically with gel formation. The coordination polymeric gel may find utility as a novel soft material in biomedical and photochemistry fields.

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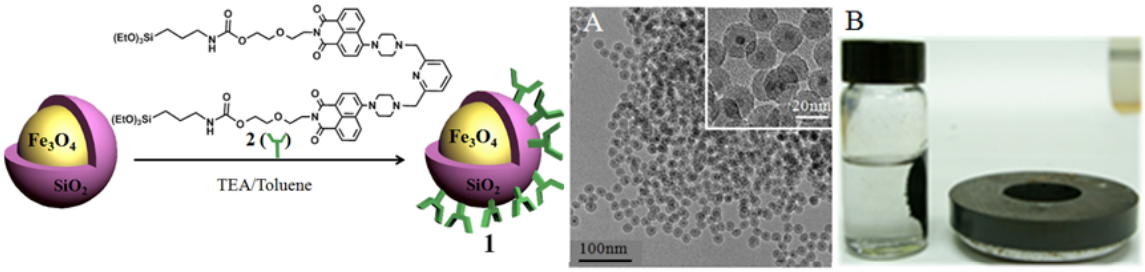
발표분야: 무기화학
발표종류: 포스터, 발표일시: 목 10:30~12:30

Preparation of Luminescent Magnetic Silica Nanoparticle for Detection of Hg^{2+} and CH_3Hg^+

박민성, *Jagadese J. Vittal, **정종화

*경상대 자연과학대학 화학과 *National University of Singapore, Singapore and Gyeongsang National Uni., Korea **경상대 화학과*

Mercury, a highly poisonous element, is a widespread pollutant which occurs from natural and anthropogenic sources. In particular, organic forms of mercury, such as methylmercury species (CH3HgX; X = halides, etc.), are much more toxic than inorganic mercury species (HgX2).1 Because of their lipid solubility, methylmercury species readily cross the blood–brain barrier, accumulate in the brain, and cause damage to the central nervous system, as well as other organs. Thus, new fluorogenic based aminonaphthalimide-functionalized $Ni@SiO_2$ and $Fe_3O_4@SiO_2$ core/shell magnetic nanoparticles 1 has been prepared, and its abilities to sense and separate metal ions were evaluated by fluorophotometry. The nanoparticles 1 exhibited a high affinity and selectivity for Hg^{2+} and CH_3Hg^+ ions over competing metal ions.



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장소: 송도컨벤시아
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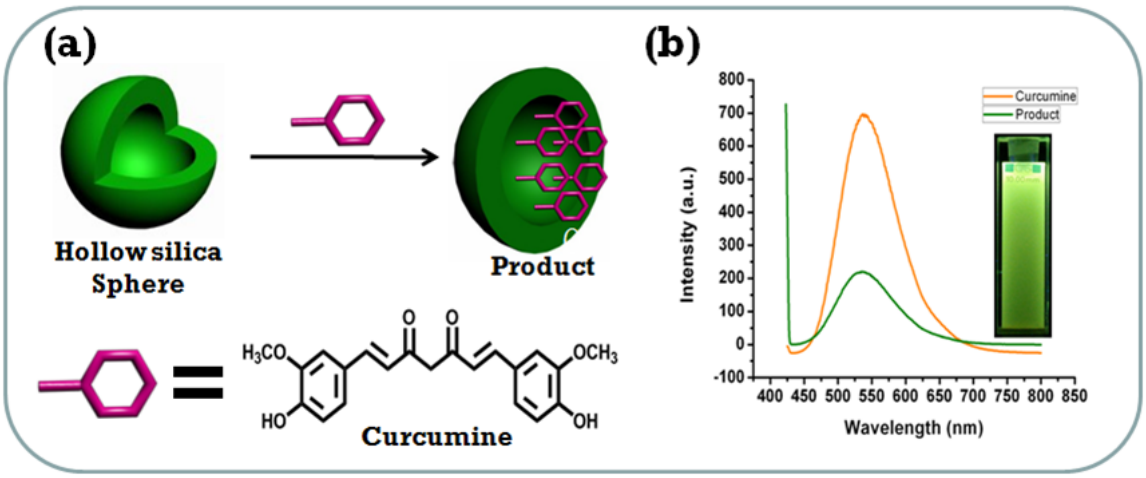
발표종류: 포스터, 발표일시: 목 10:30~12:30

Preparation of Mesoporous Type Hollow Silica Sphere By using the Self-Assembled Nanostructure

진달샘, 박경원, 서무룡, 정종화

경상대 화학과

The mesoporous hollow silica sphere(MHS) was prepared by using alanine-based amphiphile as a template. MHS was characterized by PXRD, TEM, SEM and BET isotherm analysis. MHS showed hollow structure of immobilized onto inner surface of MHS by covalent band. The curcumine attached onto the inner surface of MHS was released by change of PH into aqueous phase. We will detail discuss onto a fabrication of MHS and it's application as drug delivery system in this conference.



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Synthesis, Characterization and ROMP Activity of New Vanadium and Tungsten Complexes

Nayab Saira, 구자민, *성익경, **이효선

*경북대 화학과 *코오롱유화(주) 기술연구소 연구1팀 **경북대 자연과학대학 화학과*

New Complexes of tungsten and vanadium with tridentate ligand [O,N,O]-3-hydroxypentene-2-ylidene)amino)phenol and bidentate [O,N]-(2-pyrrolyl)methylene)-2-isopropoxyaniline are synthesized in high yield and purity. These complexes react further with alkylating reagents, which leads to the displacement of chloride ligands from the complex unit and formation of corresponding dialkyl complexes. The synthesized complexes are characterized by various spectroscopic techniques and their catalytic activity in Ring Opening Metathesis Polymerization (ROMP) of cyclic olefins in combination with Et3Al as a promoter are studied. Their efficiency in the metathesis of polar substituted monomers is low due to the interaction of monomer polar groups with catalyst components. The thermal behavior of the polymer is determined by differential scanning calorimetry (DSC) and thermogravimetric analysis (TGA) and the molecular weight of the obtained polymer is determined by GPC analysis.

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New Chiral Cu(II) and Ni(II) Complexes of Schiff's Base of Chiral Amines and Their Catalytic Application for Asymmetric Henry Reaction

Nayab Saira, *이효선, 정종화

*경북대 화학과 *경북대 자연과학대학 화학과*

Enantiometically pure substance can be synthesized by using chiral auxiliaries or chiral homogeneous catalysts. New modified chiral auxiliaries with N-(2-benzoylphenyl)-1-benzyl-1H-pyrrole-2-carboxamide, 1-benzyl-N-(1-phenylethyl)-1H-pyrrole-2-carboxamide and their NiII and CuII complexes of Schiff's base with alanine and chiral amine have been prepared in high yield and of high purity. The synthesized complexes are characterized by various spectroscopic techniques such as 1H NMR, 13C NMR IR, and UV-Visible spectroscopy. The catalytic activity of the synthesized complexes towards asymmetric Henry reaction where benzaldehyde and nitromethane in the presence of appropriate promoters are used, has been evaluated.

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Synthesis of New Ruthenium Alkylidene Complexes Via Alkylidene Exchange Reaction and Their Catalytic Activity for Ring Opening Metathesis Polymerization

우현율, *성익경, **이효선

*경북대 자연과학대학/화학과 *코오롱유화(주) 기술연구소 연구1팀 **경북대 자연과학대학 화학과*

The development of well-defined ruthenium-based complexes capable of catalyzing olefin metathesis, has been particularly focused due to their increased tolerance to functional group in the substrate. However, synthesis of the first generation Grubb's Ru catalyst is very painful with low yield due to rapid decomposition of diazomethylbenzene. Thus, ruthenium-based alkylidene complexes can be achieved by alkylidene exchange reaction. We have prepared the new series of ruthenium-based metathesis catalysts featuring imine and amine bidentate [O,N] donors and carried out the exchange reactions of alkylidene unit in the first generation Grubb's catalyst with olefinic substrate such as 1-methyl-3-vinylimidazolium iodide, 1-methyl-4-vinylpyridinium iodide and vinylpyrrole. The synthesized complexes are characterized and their catalytic activity in ROMP (Ring Opening Metathesis Polymerization) for various cyclic olefins are tested.

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Syntheses, Crystal Structures and Spectroscopic Properties of Some Metal Complexes with Polyamine Ligand

shuranjan sarkar, *홍창섭, **나명수, 이홍인

*경북대 화학과 *고려대 화학과 **한양대 응용화학과*

Polyamines have often been used as chelating ligands, forming complexes useful for catalysis, antibiotics, anti-inflammatory agents, and anticorrosion reagents. Particularly Schiff bases containing polyamines are very effective metal chelators and their metal complexes are models for a number of important biological systems. The variety of possible polyamines metal complexes with wide choice of ligands and coordination environments has incited us to take on research in this area. In this poster, we have explored some Schiff base and amide transition metal complexes those were successfully synthesized and characterized by a combination of elemental analysis, UV-vis spectroscopy, IR, EPR and x-ray crystallography.

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Metal Organic Frameworks Based on Manganese and Tricarboxylate Ligands: Syntheses and Crystal Structures

심수연, *나명수, 이홍인

*경북대 화학과 *한양대 응용화학과*

We synthesized new metal organic frameworks (MOFs) by using Mn(Ⅱ) and 1,3,5-benzenetricarboxylic acid (1,3,5-BTC) and 1,3,5-cyclohexanetricarboxylic acid (1,3,5-CTC) at different experimental conditions. Thermal decomposition of these compounds occurs at 350℃. These compounds have 3-D network structures consisting of manganese centers. Manganese is working as a node with paddle wheels of each 1,3,5-BTC and 1,3,5-CTC.

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Synthesis and Characterization of Dimethylsilyl-bridged3,4-Dimethylcyclopentadienyl/amido Zirconocenes and Titanocenes

WU CHUN JI, 구자민, *이효선

*경북대 화학과 *경북대 자연과학대학 화학과*

CGCs (Constrained Geometry Catalysts), specifically $[Me_2Si(C_5Me_4)(tBuN)]MCl_2$ (M = Ti, Zr) have received considerable attention because of distinguished chemical properties such as abnormally high activity and high thermal stability on the ethylene/a-olefin copolymerization. We have prepared dimethylsilylene-bridged 3,4-dimethyl cyclopentadienyl/amido zirconocene/titanocene complexes, $[Me_2Si(C_5H_2Me_2)(tBuN)]MCl_2$ (M = Ti, Zr) by the reaction of corresponding lithium salt of ligand with $ZrCl_4$ and $TiCl_4(THF)_2$, as metal precursors, respectively. The molecular structure of complexes $[Me_2Si(C_5H_2Me_2)(tBuN)]TiCl_2$ have been determined by X-ray crystallography. Catalytic activity of $[Me_2Si(C_5H_2Me_2)(tBuN)]MCl_2$ (M = Ti, Zr) for the ethylene/1-octene copolymerization was studied and compared with CGC in order to survey the influence of 3,4-dimethyl substituents on Cp on catalytic activity and PE properties.

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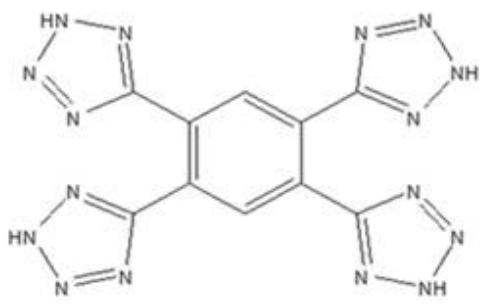
Tetrazol-based Coordination Polymeric Gel and Their Application for Chloride Anion Sensing

이혜진, *Jagadese J. Vittal, 정종화

*경상대 화학과 *National University of Singapore, Singapore and Gyeongsang National Univ., Korea*

Compound 1 has been synthesized, and it can gelatinize organic solvent such as DMF, MeOH, DMSO. 1 formed gel in the presence of Zn^{2+}, Cu^{2+}, Co^{2+}, ions without heating process. The color of the gel appeared red color due to cobalt metal ion. The red color of gel with $CoBr_2$ was changed into blue color upon the addition of Tetrabutylammonium chloride(TBACl). Added 3 equivalent TBACl, $CoBr_2$ coordination polymeric gel(CPG) color was changed from red to blue dependent upon time. Also, the red color of polymeric gel 1 was changed into blue color in the presence of Cl_2 gas. These results strongly indicate that CPG is very useful as chemosensors which can detect hamful chlorine gas.



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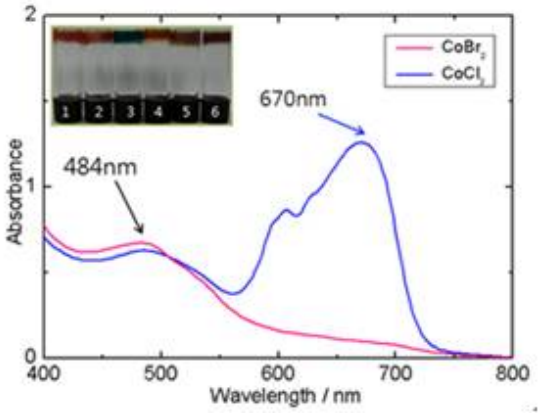

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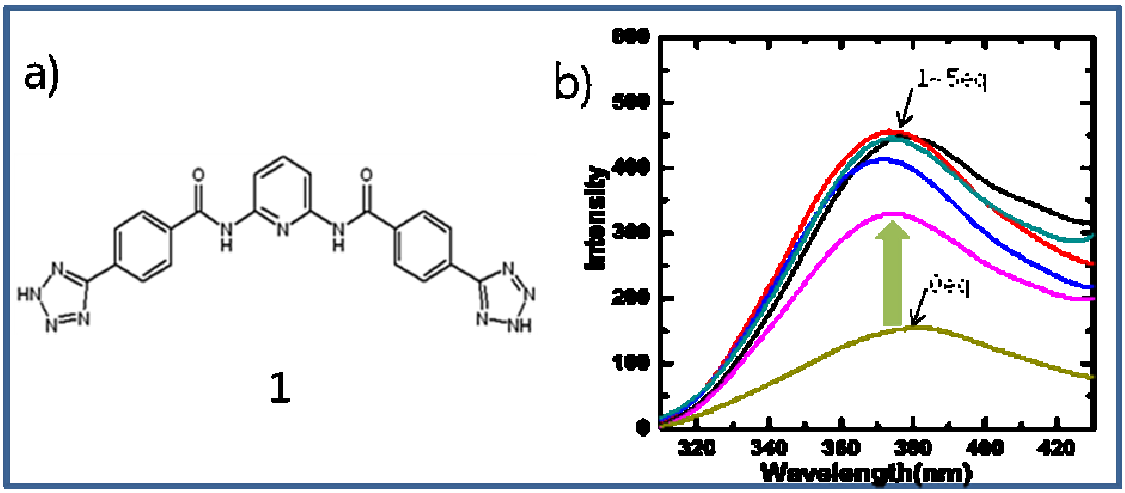
발표종류: 포스터, 발표일시: 목 10:30~12:30

Preperation of N,N'-(pyridine-2,6-diyl)bis(4-(2H-tetrazol-5-yl)benzamide)/Metal-Coordination Polymeric Gel

이지하, 서무룡, *Jagadese J. Vitta, 정종화

*경상대 화학과 *National University of Singapore, Singapore and Gyeongsang National Univ., Korea*

Compound 1 was synthesized and its gelation ability was evaluated in the absence and the presence of metal ions such as Mg^{2+}, Cu^{2+}, Zn^{2+}, Co^{2+}, Mn^{2+}, Fe^{2+}, and Cd^{2+}, in water. Interestingly, 1 formed gel in the presence of Mg^{2+}, Zn^{2+}, Cu^{2+}, and Co^{2+} ions. In addition, the coordination polymeric gel 1 with Mg^{2+} was evaluated by various anions such as NO_3^-, ClO_4^-, SO_4^{2-}, I^-, Br^- and Cl^-. The coordination gel formation of 1 is independent to anions. The freeze-dried organigel exhibits the fiber structure. UV/vis absorption studies illustrate that the hydrogel displays a typical π - π^* transition. 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 4 equivalent of Mg^{2+} ion. The results indicate that 1 forms the coordination polymeric gel by 1:4 stoichiometry. The coordination polymeric gel may find utility as a novel soft material in biomedical and photochemistry fields.



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발표분야: 무기화학
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Synthesis and Chemical Properties of New [bpmaL]MCln (M = Co, n = 2 and M = Fe, n = 2, 3) Complexes and Their Polymerization Activity for MMA

양민규, 정종화, *이효선

*경북대 화학과 *경북대 자연과학대학 화학과*

The ligands [bpmaL], which is composed of N,N-Pyrazolylmethylaniline moiety, have been successfully coordinated to the cobalt and iron metal to give [bpmaL]MCln (M = Co, n = 2 and M = Fe, n = 2, 3). Interestingly, all complexes are very air stable and very inactive for a-olefin polymerization as a catalyst for cationic addition polymerization in metal center. However, [bpmaL2]CoCl2, where [bpmaL2] is N,N-Bis{(1-pyrazolyl)methyl}-2,4,6-trimethylaniline, have shown catalytic activity of polymerization for MMA (Methyl methacrylate) in the presence of MAO to give PMMA. Thus, synthesis, characterizations and their chemical reactivity of these complexes and polymerization of MMA using these complexes, are studied.

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The helicity of helical silica nanotube from optical purity of chiral gelator

오채영, 이미성, *문해경, 한현주, **진종성, **정의덕, 정옥상

*부산대 화학과 *한국기초과학지원연구원 하이테크소재연구부 **한국기초과학지원연구원 하이테크부품소재연구지원센터*

We synthesized helical silica nanotube using neutral and ionic organogelators. The neutral gelator determines the shape of morphology, and the ionic gelator covers to the neutral gelators for the connection of silica oxide compounds. We studied an effect of helicity for preparation of helical silica nanotubes as control of optical purity to the neutral gelator. Under the experiment results, the helicity of the silica nanotubes were cleared when using the highest optically pure neutral gelator.

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Anion effects on construction of Zn(II) compounds with a chelating ligand bis(2-pyridylmethyl)amine (bispicam) and their catalytic activities

엄근희, 박현민, *김진훈, 이홍규, **장승표, **김철, ***김성진, ****김영미

*서울산업대 정밀화학과 *서울산업대 생무기연구실 **서울산업대 정밀화학과 친환경소재제품센터 ***이화여대 화학과 ****이화여대 화학-나노과학과*

Complexes of the general formula [Zn(bispicam)2]X2 (X = Cl-, Br-, I-, NO3-, ClO4-, benzoate, and OTf-) have been obtained, and there were fac geometric isomers (a) or enantiomers (c) and (d) according to anions. Interestingly, complexes 4 - 6 with geometric and enantiomeric isomers did form mononuclear complexes without H-bonding, whereas 1-3 with only facial isomer formed polymeric compounds via hydrogen bonding interactions. Moreover, complexes 4 - 6 could carry out the catalytic transesterification of a range of esters with methanol under the mild conditions. Importantly, the catalyst 4B with an unsaturated structure has shown better efficiency than the catalysts, 4A, 5, and 6, having saturated structures. To explain this reactivity difference, two different reaction mechanisms have been proposed (metal-based vs. amide N-H-based).

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Efficient Olefin Epoxidation by Robust Re4 Cluster-Supported MnIII Complexes with Peracids: Evidence of the Multiple Active Oxidants, MnV=O, MnIV=O, and MnIII-OO(O)CR Species, That Operate Simultaneously

송영주, *박현민, *이주훈, *조영단, **이정아, 김철, ***김성진, ****김영미

*서울산업대 정밀화학과 친환경소재제품센터 *서울산업대 정밀화학과 **서울산업대학원 정밀화학과 ***이화여대 화학과 ****이화여대 화학-나노과학과*

Two new tetranuclear chalcocyanide cluster complexes, [{Mn(saloph)H2O}4Re4Q4(CN)12]•4CH3OH•8H2O (saloph = N,N'-o-phenylenebis(salicylidenaminato), Q = Se (1-Se), Te (2-Te)), have been synthesized by the diffusion of a methanol solution of [PPh4]4[Re4Q4(CN)12] in a methanol solution of [Mn(saloph)]+. The structure of 2-Te was determined by X-ray crystallography. These rhenium cluster-supported [MnIII(saloph)] complexes catalyzed efficiently a wide range of olefin epoxidation upon treatment with meta-chloroperbenzoic acid (MCPBA), under mild experimental conditions. Olefin epoxidation by these catalysts was proposed to involve the multiple active oxidants MnV=O, MnIV=O, and MnIII-OO(O)CR. Evidence for this approach was derived from reactivity and Hammett studies, H218O-exchange experiments, and the use of peroxyphenylacetic acid as a mechanistic probe. Moreover, it has been observed that the participation of MnV=O, MnIV=O, and MnIII-OOR can be controlled by changing the substrate concentration. This mechanism provides the greatest congruity with related oxidation reactions by using certain Mn complexes as catalysts.

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Assembly and Characterization of Porphyrin-Viologen Dyads with Cucurbit[n]uril (n= 7, 8)

김민경, 이민정, 김희준

금오공과대 응용화학과

The chemistry related to porphyrins and metalloporphyrins was well studied in past and it is imperative to mention these compounds are well used in formation of photosynthetic materials because of their unique structures and rich photoelectronic properties. In the mimics of photosynthetic materials, porphyrins and metalloporphyrins act as light harvesting units and as electrons donor while methylviologen (N,N-dimethyl-4,4-bipyridinium, MV2+) is a common electron acceptor in electron transfer reactions. The inclusion complexes of methylviologen dication in larger cucurbit[n]uril homologues (CB[n], n = 7 and 8), are thermodynamically and kinetically stable. Furthermore, inclusion behaviors coupled with the redox chemistry of methylviologen in CB[7] and CB[8] can also form stable inclusion complexes with cation radical (MV+.). Thus, we have been interested in supramolecular manipulation of photoinduced electron transfer processes in porphyrin-viologen dyads with cucurbit[n]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 synthesis of porphyrin-viologen dyad, its inclusion behaviors in CB[n] (n = 7, 8), and their spectroscopic properties.

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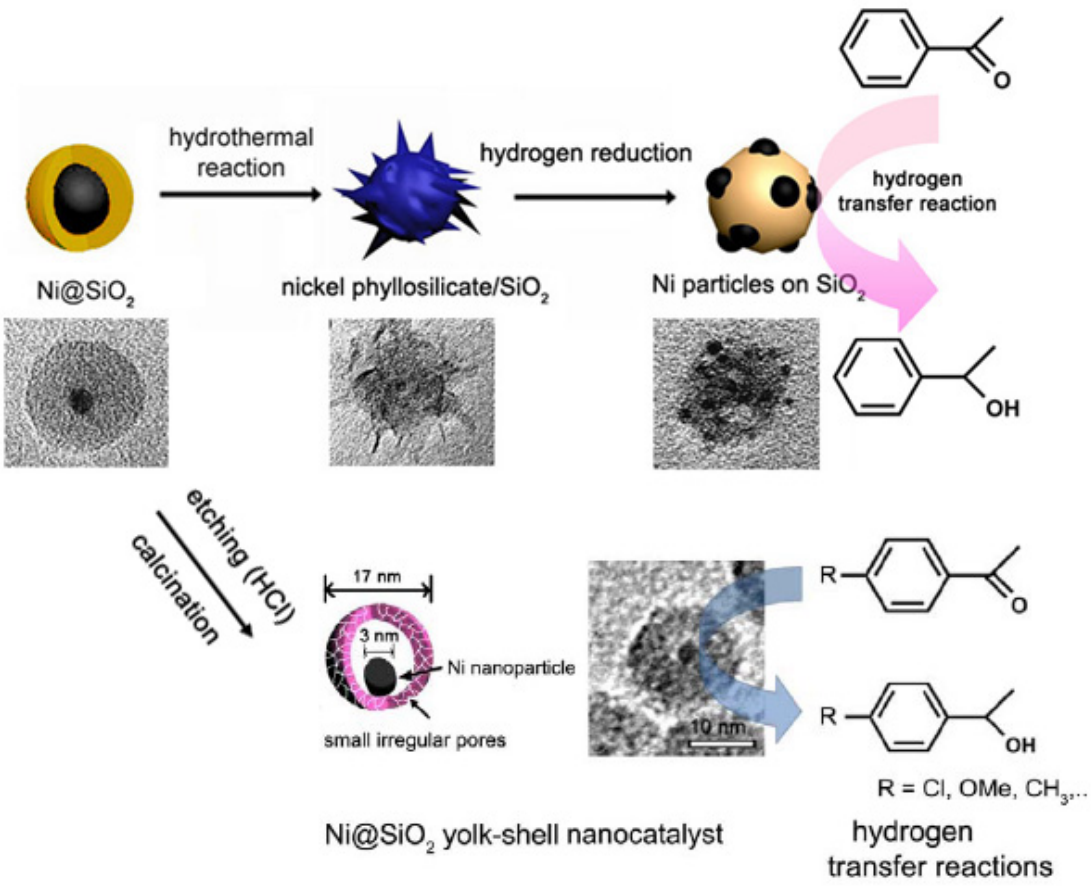
발표종류: 포스터, 발표일시: 목 10:30~12:30

Catalytic Hydrogen Transfer of Ketones over Nickel-Silica Hybrid Nanostructures

박지찬, *이현주, *박강현, 송현준

*KAIST 화학과 *부산대 화학과*

In the present work, we report the synthesis of nickel-silica hybrid nanocatalysts that bear tiny nickel particles with an average diameter of 3 nm. The nickel nanoparticles were coated with silica through the microemulsion method. The resulting Ni@SiO_2 core-shell nanoparticles were subsequently transformed to Ni particles on silica spheres via a branched nickel phyllosilicate phase by hydrothermal and hydrogen reduction reactions. In addition, the Ni@SiO_2 core-shell nanoparticles could be also partially etched by acid treatment and the sequential calcination process of the particles yielded yolk-shell nanocatalysts with a uniform structure. The hybrid particles with different morphology were employed as active nanocatalysts for heterogeneous hydrogen transfer reactions of acetophenone.



THE KOREAN CHEMICAL SOCIETY

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발표코드: **Ⅰ33P37포**
발표분야: 무기화학
발표종류: 포스터, 발표일시: 목 10:30~12:30

Controlled Synthesis of Copper Nanowires via Hydrothermal Reaction of Copper Salt and Long Alkylamine

이정인, 박수진

울산과학기술대 에너지공학부

Copper wires can be used as a wide variety of applications, like chemical sensors, catalyst, and interconnects. In this study, copper nanowires were prepared via hydrothermal reaction of Cu (II) and long alkylamine at 160 – 210 ^{o}C. Recently, hydrothermal process has been widely used to synthesize nanostructured materials. In this study, we investigated the effect of alkyl chain length, reaction temperature, and amount of alkylamine relative to copper (II) on the length and diameter of as-prepared copper nanowires. Furthermore, as-prepared copper nanowires were transformed to copper oxide by a simple thermal oxidation process that was carried out at 400 ^{o}C for 1 hr. Copper and copper oxide nanowires were characterized by scanning electron microscopy, transmission electron microscopy, X-ray powder diffraction and energy dispersive X-ray patterns. These results indicate that as-prepared copper nanowires are single-crystalline and grown along with the direction of .

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Synthesis and Characterization of Tin(IV) Porphyrin Axially Coordinated by Zinc Porphyrins with Fluorene Groups as Light Harvesting Complex

박수영, 이기선, 김희준

금오공과대 응용화학과

It will not be wrong to say, “Nature a big reaction pot” where numbers of reactions always take place in reversible or irreversible modes. Among all these reactions, the photosynthesis, where synthesis of wide varieties of organic matters is accomplished, proceeds in presence of sunlight by using chlorophyll as a light harvesting complex of plants. Chlorophyll is a analogue of porphyrin. Porphyrins and metalloporphyrins are well known as photosensitizer and used in solar energy conversion. Herein, we present the synthesis of tin(IV) porphyrin-zinc porphyrins complex which involves zinc porphyrins with fluorene groups as axial ligands on the tin(IV) porphyrin.

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Photocatalytic Activity of Porphyrin-Polyoxometalate Hybrid Nano-Materials

Changhong Li, 김희준, *최원용

*금오공과대 응용화학과 *포항공과대 환경공학부*

Porphyrins and metalloporphyrins, the synthetic structural analogue of chlorophyll in plant photosynthesis, have been widely investigated for their photochemical activity for various applications such as environmental photocatalysis, hydrogen production, and solar cell. On the other hand, polyoxometalates (POMs) are the inorganic equivalent of a porphyrin. POMs are discrete metal oxide clusters that are ca. 1 nm in diameter and can have a variety of compositions. We have recently synthesized porphyrin-polyoxometalate hybrid nano-materials by ionic self-assembly of Sn(IV)-porphyrin cations and polyoxometallates anions in aqueous solution. The hybrid nano-materials (SnP-POM) were characterized by various spectroscopic and microscopic techniques. Sn-POM is feasible in visible light-sensitized photocatalysis for the hydrogen production from water. Here we present the synthesis, characterization and photocatalytic activity of SnP-POM in detail.

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발표종류: 포스터, 발표일시: 목 10:30~12:30

Recognition of Amine Cations by Tin(IV) Porphyrins

이미희, 김희준

금오공과대 응용화학과

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

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발표종류: 포스터, 발표일시: 목 10:30~12:30

Synthesis, crystal structures, photoluminescence, and catalytic reactivity of novel coordination polymers (0-D, 1-D to 2D) constructed from cis-1,2-cyclohexanedicarboxylic acid and various bipyridyl ligands

유승만, *장승표, *엄근희, *이홍규, *조영단, 김철, **김성진, ***김영미

*서울산업대 정밀화학과 친환경소재제품센터 *서울산업대 정밀화학과 **이화여대 화학과 ***이화여대 화학-나노과학과*

Six Zn(II)-(e,a-cis-1,2-chdc) complexes, [Zn2(1,2-chdc)2(2,2'-bpy)2(H2O)2] 1, [Zn2(1,2-chdc)2(H2O)(μ-bpa)]n 2, [Zn2(μ-1,2-chdc)2(μ-4,4'-bpy)]n 3, [Zn2(μ-1,2-chdc)2(μ-bpe)]n 4, [{Zn2(μ-1,2-chdc)2}n-(μ-bpe)-{Zn2(μ-1,2-chdc)2(H2O)2}]n 5, and [Zn(μ-dtp)(μ-1,2-chdc)]n 6 (1,2-chdc = 1,2-cyclohexanedicarboxylate), with different assistant ligands (2,2'-bipyridine (2,2'-bpy), 1,2-bis(4-pyridyl)ethane (bpa), 1,2-bis(4-pyridyl)ethylene (bpe), 1,3-bis(4-pyridyl)propane (bpp), and, 4,4'-bipyridine (4,4'-bpy) and 4,4'-dithiodipyridine (dtp)) have been synthesized and their structures were determined. Depending on the assistant ligands, the structures and dimensionalities of Zn(II)-(e,a-cis-1,2-chdc) complexes has been varied. Two carboxylates in e,a-cis-1,2-chdc coordinate to Zn(II) ions with (11) or (10) connectivity. Photoluminescence study of the compounds 1-6 showed that emission spectra of compounds 1, 2, 4, and 5 were observed at 343 nm for 1, 419 nm for 2, 507 nm for 4, 396 nm for 5, respectively, while no obvious luminescences were displayed for 3 and 6. In addition, it has been found that compound 1 catalyzed the transesterification reaction of phenyl acetate with methanol, with quantitative conversion to methyl acetate, under the neutral conditions, while compounds 2 - 6 showed very slow conversions. The thermal stabilities of these complexes were also examined.

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발표종류: 포스터, 발표일시: 목 10:30~12:30

Synthesis of InP/ZnS nanocrystal quantum dots using single source precursors

정소명, *정소희

*충북대 화학과 *한국기계연구원 나노기계연구본부*

Semiconductor nanocrystal quantum dots (NQDs) have attracted attention as they can be applied in various areas such as LED, solar cell and biological imaging, and so on. For practical reason, there is a need for a method that provides rapid and efficient production of highly luminescing nanocrystals without toxic elements such as cadmium or lead. In this study, an efficient and rapid method of producing InP/ZnS nanocrystal quantum dots with high quantum yield (~ 60 %) using single source precursor will be presented. Synthesis was carried out stepwise-InP core formation followed by the epitaxial coating. Resulting quantum dots luminesce in the visible wavelength with full width of half maximun (FWHM) less than 40 nm.

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발표종류: 포스터, 발표일시: 목 10:30~12:30

Synthesis of $Cu(In_xGa_{1-x})Se_2$ nanoparticles through a simple sonochemical method

황차환, 심일운

중앙대 화학과

Synthesis of $Cu(In_xGa_{1-x})Se_2$ nanoparticles through a simple sonochemical method were tried in various solvents under the multibubble sonoluminescence (MBSL) conditions. For the synthesis, we used copper nanoparicles or $CuCl_2$, $InCl_3$, $GaCl_3$ and Se powder. Methanol was used as solvent with ethylenediamine. The prepared $Cu(In_xGa_{1-x})Se_2$ nanoparticles are examined by XRD, ICP, UV-Vis spectrophotometer, and HR-TEM.

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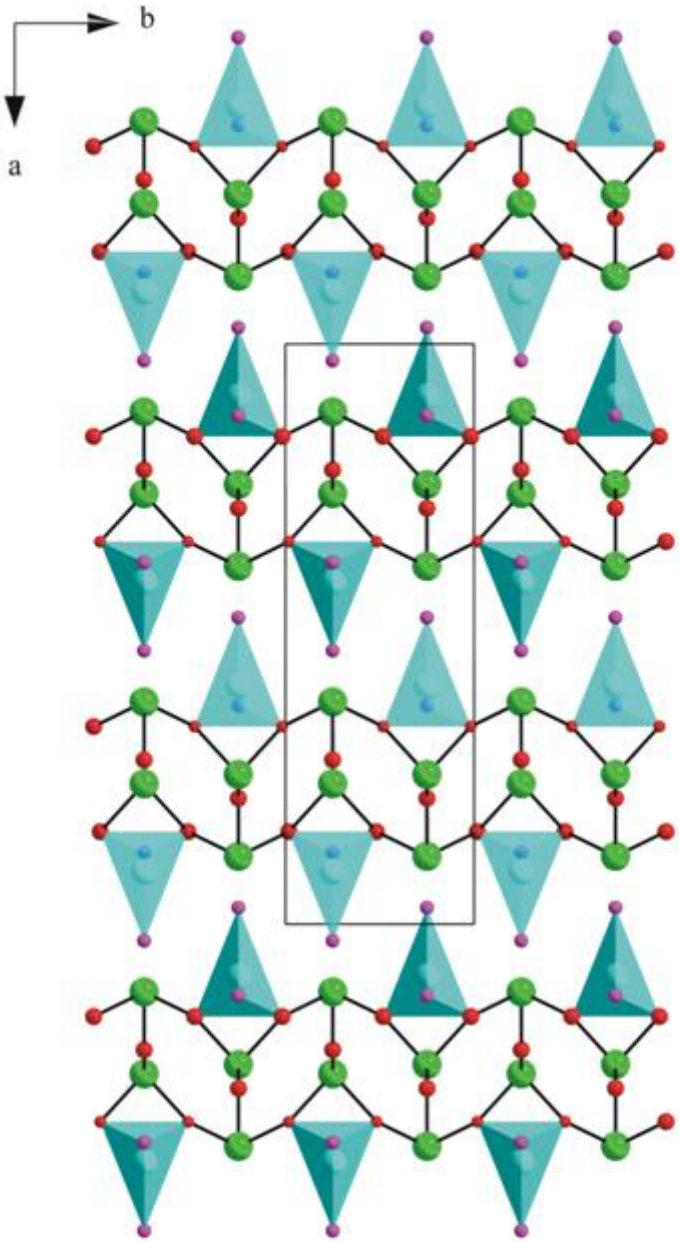
발표종류: 포스터, 발표일시: 목 10:30~12:30

Lone Pairs as Chemical Scissors in New Antimony Oxychlorides, $Sb_2ZnO_3Cl_2$ and $Sb_{16}Cd_8O_{25}Cl_{14}$

조빛나, 김민경, 이동우, 옥강민

중앙대 화학과

Two new metal antimony oxychlorides, $Sb_2ZnO_3Cl_2$ and $Sb_{16}Cd_8O_{25}Cl_{14}$ have been synthesized by solid-state reactions using Sb_2O_3 and $ZnCl_2$ (or $CdCl_2$) as reagents. The structures of $Sb_2ZnO_3Cl_2$ and $Sb_{16}Cd_8O_{25}Cl_{14}$have been determined by single-crystal X-ray diffraction. Both the reported materials contain Sb^{3+} cations that are in asymmetric coordination environment attributable to their stereoactive lone pair. $Sb_2ZnO_3Cl_2$ has a novel two-dimensional layered structure consisting of distorted ZnO_2Cl_2 tetrahedra and SbO_3 polyhedra. $Sb_{16}Cd_8O_{25}Cl_{14}$ exhibits a one-dimensional structure consisting of Sb^{3+}–Cd^{2+}–oxide rods, Cd^{2+}–chloride double chains, and isolated Cl^- ions. Complete separation of the halophile and the chalcophile moieties are observed from the reported materials. Detailed structural analysis, Infrared spectra, thermogravimetric analysis, ion-exchange reactions, and dipole moment calculations are also presented.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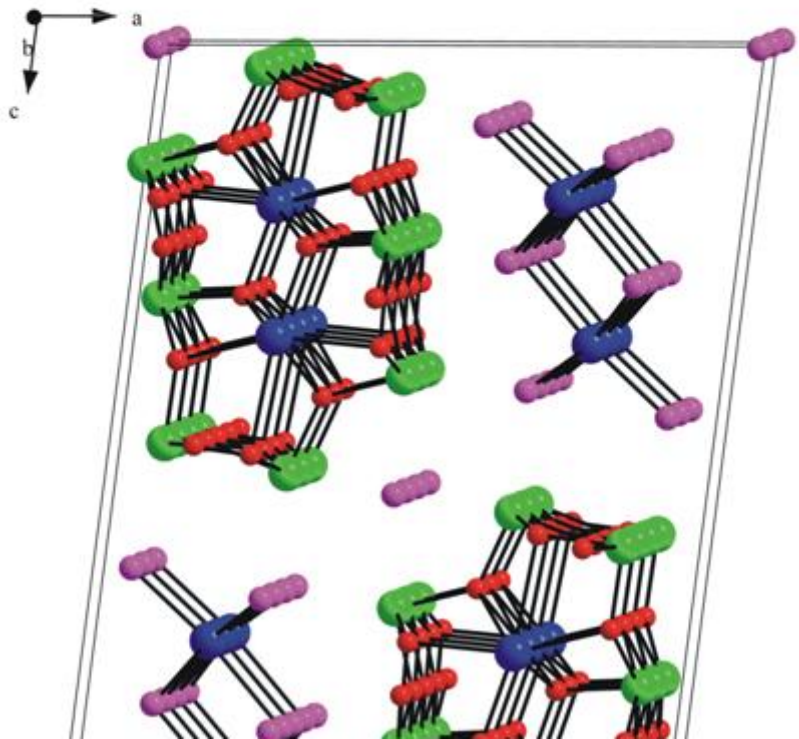
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대한화학회
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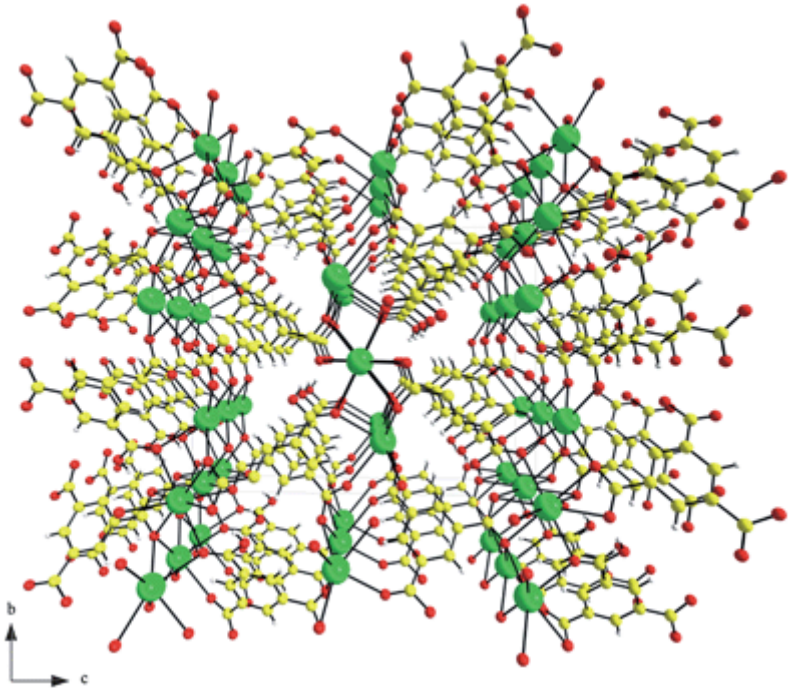
New tubular alkali metal-organic framework materials, $A_3[C_6H_3(CO_2)(CO_2H_{0.5})(CO_2H)]_2$ (A= K or Rb)

김민경, 조빛나, 이동우, 심일운, 옥강민

중앙대 화학과

Two new tubular alkali metal-organic framework materials, $A_3[C_6H_3(CO_2)(CO_2H_{0.5})(CO_2H)]_2$ (A=K or Rb) have been synthesized through solvothermal reactions using NH_4F, 1.3.5-$C_6H_3(CO_2H)_3$, ANO_3, and N,N-Dimethylformamide at 180℃. The structure has been determined by single-crystal X-ray diffraction. $A_3[C_6H_3(CO_2)(CO_2H_{0.5})(CO_2H)]_2$ have novel tubular structures consisting of channels of AO_6 and AO_8 alkali metal oxide groups as well as the benzenetricarboxylate organic linker. Detailed structural analysis with full characterization including infrared spectra, thermogravimetric analyses, and elemental analyses are reported. Crystal data of the $C_{18}H_9K_3O_{12}$: monoclinic, $P2_1/c$ (No.14), a=3.9802(8)Å, b=13.615(3)Å, c=17.671(4)Å, Crystal data of the $C_{18}H_9Rb_3O_{12}$: monoclinic, $P2_1/c$ (No.14), a=4.0727(8)Å, b=13.897(3)Å, c=17.853(4)Å.



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발표종류: 포스터, 발표일시: 목 10:30~12:30

A study on the properties of ITO thin films by Roll-to-Roll sputter

김정수, *강보갑, 박미영, *김후식, *임우택, *최식영

*안동대 화학과 *안동대 응용화학과*

Indium tin oxide(ITO) thin films were deposited on polyethylene terephthalate(PET) substrates by D.C. magnetron roll-to-roll sputter system with In2O3(95 wt%) - SnO2(5 wt%) target at room temperature. In this experiment, the influence of D.C. power, winding speed, and oxygen flow rate on electrical and optical properties of ITO thin films were investigated with the results of sheet resistance, transmittance, and chromaticity(b*). As a result, the chromaticity (b*) and transmittance of the ITO thin films were broadly dependent on the thickness and O2 flow rate. High quality ITO films with sheet resistance of 416 ohm/square, transmittance of 88.73%, and chromaticity(b*) of 2.83 were able to be formed at D.C. power of 600W, winding speed of 0.56 m/min, and O2 flow rate of 1.4 sccm. The four point probe and spectrophotometer are used to investigate the properties of ITO thin films.

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A New Approach to Immobilize Single DNA Molecule at the Apex of AFM Tips for Single Molecule Dynamic Force Microscopy

김덕회, 김정숙, 박준원

포항공과대 화학과

In this report, we suggest a new approach to immobilize single molecule at the apex of AFM tips. We employed dendron-modified AFM tips and substrates to pick the single DNA only. Modification with a cone-shaped dendron has created ample lateral spcing, and enabled us to pick a single molecule with an atomic force microscope (AFM). Furthermore, the picked single DNA was used as a template to introduce a single new DNA covalently at the end of a single probe DNA which was hybridized with the picked DNA. The existense of the covaletly linked new single DNA was confirmed by force measurements on generic sufraces.

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New type of the guadinate based Tantalum complexes: Potential precursors for tantalum nitride MOCVD

민재기, 김창균, 정택모

한국화학연구원 화학소재연구단

Tantalum nitride (TaNx) films have been an attractive candidate as a diffusion barrier for copper-interconnect technologies because of their high thermal, mechanical, chemical stability, and good electrical conductivity.Herein for the first time, we report the syntheses and characterization of guadinate based tantalumcomplexes.

한국화학회 THE KOREAN CHEMICAL SOCIETY

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Desolvated Structures and Gas Sorption Properties *versus* Activation Methods of a Porous Metal–Organic Framework

박혜정, 임대운, 백명현

서울대 화학부

A Zn_4O-based MOF has been prepared by using an elongated carboxylate organic building block to obtain large surface area and pore volume. Despite the large void space, the MOF shows single-crystal to single-crystal transformations on guest exchange and on various desolvation processes such as room temperature evacuation, high temperature evacuation, and supercritical drying. In this presentation, we will show for the first time how the activation methods affect the desolvated structures and the gas sorption properties of the MOF.

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Selective carbon dioxide adsorption in noble 2-D coordination polymer

허정석, 김정권, 박균하, 박윤봉

충남대 화학과

Highly porous coordination polymers are promising candidates for many applications including separations, catalysis, optical devices, and even electronic devices. One important target is development of selective carbon dioxide adsorbent. We prepared noble 2-D coordination polymer by assembling functionalized phthalic acid moiety and copper (II) ions. The building blocks bridge in-between copper ions forming paddle-wheel type of bimetallic centers and it gave highly porous 2-D network structure eventually. The window size of cavities in the network matches well with that of carbon dioxide and selective gas uptake was observed. We will present X-ray crystal structure and gas sorption results of the noble network.

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Direct Dizinc Displacement Approach for Efficient Detectionof Cu2+ in Aqueous Media: Acetate versus PhenolateBridging Platforms

강지나, *D.G.Churchill

*KAIST 화학과 *KAIST 화학과*

Two chiral and one racemic fluorescent dimeric zinc complex {[Zn2(slysH)2Cl2]·(CH3OH)2·(H2O)3(1), [Zn2(slysH)2 (NO3)2]·(H2O)3 (2), [Zn2(rslysH)2(μ-OAc)2] (3)} are compared herein. Presently,3 has been synthesized by a one-pot reaction in which the D-/L- lysine-based Schiff base ligand10 [slys = 6-amino-2-{(2-hydroxybenzylidene)amino}hexanoate] is generated in situ. Thesecompounds have been characterized by single-crystal X-ray diffraction and by variousspectroscopic techniques. The structures of previously reported compounds 1 and 2 are closelyrelated in which two zinc centers possess two phenolate-bridges and an axial chloride or nitrateligand. The novel compound 3 differs structurally through the presence and coordination mode of15 two bridging acetate groups spanning the dizinc core and formally releasing the phenolate bridgingSchiff base ligands. These compounds (1 - 3) are highly blue fluorescent, either as solids ordissolved species. Under neutral and aqueous conditions (pH 7.4; 0.01 M HEPES buffer,H2O:MeOH = 9:1), the quantum yields are ΦF = 0.17 (1), 0.21 (2) (λex = 352 nm, λem = 452 nm),ΦF = 0.16 (3) (λex = 354 nm, λem = 452 nm). Complex 3 metal ion detection capability (i.e., Na+,20 K+, Ca2+, Mg2+, Co2+, Ni2+, Mn2+, Cu2+, Pb2+, Ag+, Hg2+, and Cd2+) was gauged in aqueous mediaat physiological pH facilitated by the similarity of its starting photophysical properties with thoseof 1 and 2. These dizinc species were all found to act as a highly selective fluorescent ON-OFFprobes for Cu2+ through the direct displacement of two zinc ions in aqueous media at physiologicalpH range. The phenolate-bridged compounds 1 and 2, however, showed better selectivity towards25 Cu2+ over competitive ions, Ni2+ and Co2+ than the acetate-bridged compound 3.

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Two isomers containing a [Cu(Me_2bpzb)] unit: molecule (0-D) and 1-D

이주훈, *송영주, *유승만, **김진훈, *김철, ***김성진, ****김영미

*서울산업대 정밀화학과 *서울산업대 정밀화학과 친환경소재제품센터 **서울산업대 생무기연구실 ***이화여대 화학과 ****이화여대 화학-나노과학과*

Two isomers (molecule 1 and 1-D 2) containing [Cu(Me_2bpzb)] units have been obtained under the different reaction conditions, and their structures have been determined by X-ray crystrallography. From the temperature-dependent magnetic data for 2, there was no interaction between Cu^{2+} ions through the ligand. The photoluminescence of the free H_2Me_2bpzb molecule displayed an intense emission band centered at about 482 nm, while complexes 1 and 2 exhibited no obvious emission bands. Moreover, a new and mild catalytic system for the effective aerobic oxidation of benzyl alcohol to benzaldehyde has been developed.

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발표종류: 포스터, 발표일시: 목 10:30~12:30

Detection of Ammonia based on Fluorophore Coordinated Metal Complex

김지연

국민대 생명나노화학과

Recently, many people have been interested in atmospheric pollution and toxic gas. It is necessary to develop the sensing system to detect these harmful chemicals. Especially ammonia gas is a basic material which stimulates the body tissues and smells bad. Due to these reasons, the legally permitted concentration is regulated up to 50 ppm. However, ammonia gas is a material which is discharged while driving the automotive and from the refrigeration system. Also, the ammonia is synthesized in large quantities in the chemical industry. Therefore, the measurement of atmospheric ammonia concentrations is necessary, leading researches on ammonia gas sensors. Currently, solid-state gas sensors, conducting polymer gas sensors, mixed oxide gas sensors, amperometric gas sensors, catalytic field-effect devices, optical gas analyzers are already under active progress.However, when very low concentrations are to be measured, solid-state ammonia sensors are not sensitive and selective enough. Optical methods that make use of lasers are often expensive and large. The detecting way of other sensors has showed not only low sensitivity but also involve indirect measurement principles.Herein, we invented the fluorophore-containing complex sensor for the direct detection with high sensitivity. The fluorescence of fluorophore is quenched by Photoinduced Electron Transfer (PET) mechanism and upon addition of ammonia the fluorescence intensity dramatically increases. In future, the system may be applied to environmental, automotive and medical applications. Acknowledgement : *This work was supported by a grant from the Fundamental R&D Program for Core Technology of Materials funded by the Ministry of Knowledge Economy, Republic of Korea*

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Tuning of the Size of Vanadium Oxide Nanocrystals, Using Tailored Sol-gel Processes

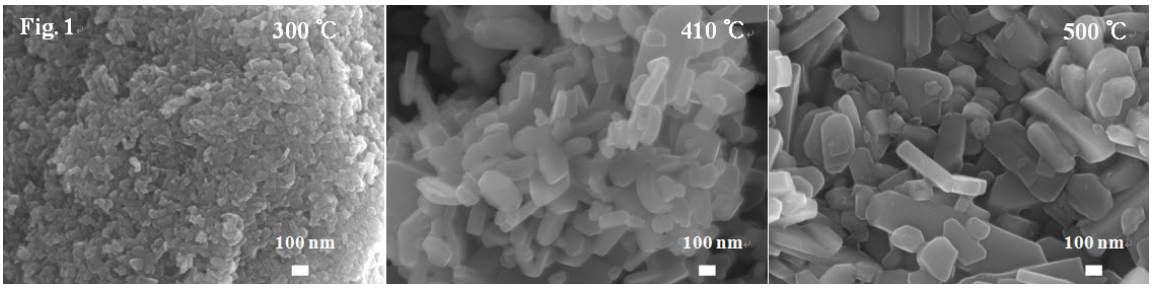
이경훈, *윤성호

*국민대 나노과학기술협동과정 *국민대 생명나노화학과*

Nanomaterials have been attractive for their unique properties to be used as building units in bottom-up process. Among valuable nanomaterials, vanadium oxide nanocrystals are of interest due to their various applications as catalyst, cathode material in high-energy lithium batteries, and material in electric field-effect transistors. The controllability in size of vanadium oxide is a key issue to employ them in each field, because the wide application can be realized only with size-tuned specific materials. Recently, Kang and his coworkers demonstrated the technique to synthesize vanadium dioxide on sapphire by sol-gel method [1] and the methods to prepare vanadium oxide nanocrystals have been reported by Do's group [2]. However, the size of vanadium oxide nanomaterials has ever been controlled yet, as we acknowledged. Herein, we present the preparation of $V_2O_{4.6}$ nanocrystals by the sol-gel processes and the tuning of the size of these nanocrystals by varying control factors, such as temperature and concentration. (Fig. 1)

Reference[1] Chae, B. G.; Kim, H-T.; Yun, S-J.; Kim, B-J.; Lee, Y-W.; Youn, D-H.; Kang K-Y. *Electrochem. Solid-State Lett* . 2006, 9, C12. [2] Nguyen, T-D.; Do, T-O. *Langmuir* . 2009, 25, 5322.

Acknowledgement : This work was supported by the Korea Science and Engineering Foundation (KOSEF) grant funded by the Korea government (MEST)



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Theoretical and Experimental Studies of the Photo-induced Electron Transfer between Amines and the BODIPY Dye: Way to Develop Formaldehyde Fluorescent Sensor.

송혜선, 윤성호, *박규순

*국민대 생명나노화학과 *국민대 화학과*

Fluorescent sensors are of interest in the field of specific pollutants detection, biochemistry, and neuro-science. One of the frequently used tactics to develop such sensors is fluorescent quenching by lone pair electron of amine, so called photoinduced electron transfer mechanism. Very few reports are there about little theoretical backgrounds on diverse fluorphore. We aim to provide information about correlation of the photo-induced electron transfer between electron density of nitrogen in amines and the BODIPY dye using computation chemistry together with experimental approach. These compounds, shown in Figure 1, were prepared and their fluorescent characters are confirmed (Figure 2). Molecular orbital energies of each compounds were calculated using B3LYP/6-31G(d) method and intensity of fluorescence is predicted as in following order (compound AB I > AB II > AB III), which is in good agreement with experimental results. Herein, we present the theoretical background on the phenomenon that tertiary amine compound, AB III, are less fluorescent compared with primary and secondary amine compounds, AB I and AB II.

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Preparation of RuO2 Thin Film Using Cyclic Voltammetry.

전여진, 윤성호

국민대 생명나노화학과

Owing to the extensive use of fossil fuel, the concentration of carbon dioxide in air has been increased, causing green house effect. If such trend continues, the amount of fossil fuel reserved on Earth will be depleted within 40~60 years. Therefore, we need to develop alternative energy sources. Among alternative sources, hydrogen gas is a premising candidate because hydrogen energy obtained from the decomposition of water using incessant solar energy returns to harmless water molecule again via combustion without involvement of any carbon atoms. To this end, we have continuously searched for good catalysts for water oxidation. Conductive and relatively robust ruthenium dioxide (RuO_2) have been used as one of best water splitting catalysts. Currently, ruthenium dioxide is often prepared by sol-gel, micro emulsion, and electro deposition method. Herein, we demonstrated the direct formation of ruthenium dioxide thin film on titanium substrate with cyclic voltammetry(CV). To control the morphology of surface and thickness, we regulate sweep rate and cycle numbers in CV. Characterizations, including surface roughness and thickness, are performed by scanning electron microscopy(SEM), atomic force microscopy(AFM), and X-ray diffraction methods.Acknowledgement : This work was supported by the KRCF (Korea Research Council of Fundamental Science & Technology) and KIST (Korea Institute of Science & Technology) for “National Agenda Project Program”

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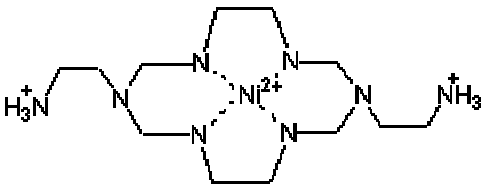
Hydrogen bonding incorporated self-assembly of a nickel(II) complex of protonated macrocycle with square planar complexes

김성민, *정민철, **곽지훈

*순천대 화학전공 *순천대 화학공학과 **순천대 화학과*

Usually, the strategy for the design and construction of the self-assembly structure with macrocyclic complexes has been focused, but even, limited on tuning two-axial sites of the complexes with different auxiliary ligands. Recently, the combination of coordination and hydrogen bonding approach has provided particularly interesting supramolecular systems in metal-organic hybrids. Here we explore the development of a building block containing potentially coordination and hydrogen bonding sites as well to evaluate the role of hydrogen bonding in self-assembly of tetraaza donor macrocyclic complex. We used a polyazamacrocyclic complex of nickel(II) ([Ni(H2L)]4+, where L = 1,8-bis(2-aminoethyl)-1,3,6,8,13-hexaazacyclotetradecane), in which two protonated 2-aminoethyl groups are attached to the bridgehead nitrogen atoms as a cationic building block. And appropriate square-planar complexes used as anionic building blocks



$[Ni(H_2L)]^{4+}$

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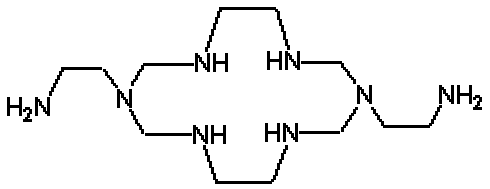
Preparation and properties of self-assembled structures by the combination of hexaazamacrocyclic complex of nickel(II) and tetracyanonickelate(II)

김성민, *곽지훈

*순천대 화학전공 *순천대 화학과*

Polyazamacrocyclic complexes of nickel(II) have been used as elegant building blocks to produce self-assembled structure with specific network topologies from one-dimensional chains to three-dimensional interwoven open framework as well as with potentially interesting properties such as ion-exchange, molecular adsorption, magnetic interaction. Here, we used [M(L)]2+ and [M(H2L)]4+, where M= Ni or Cu and L = 1,8-bis(2-aminoethyl)-1,3,6,8,13-hexaazacyclotetradecane, as cationoic building blocks for the construction of suramolecules. In this presentation, the properties and topologies of obtained products will be discussed in detail



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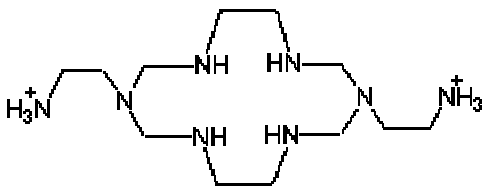

H_2L

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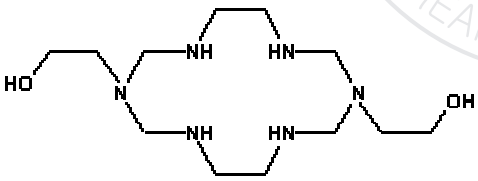
Design and preparation of self-assembled structure with hexaaza macrocyclic complexes and btca.

엔크줄, *정민철, 곽지훈

*순천대 화학과 *순천대 화학공학과*

Two novel complexes of composition with Cu(L)btca2- (1) and Ni(L)btca2- (2) were obtained by the reaction of [M(L)]2+(where M = Ni or Cu) and btca (=1,2,4,5-benzenetetracarboxylic acid), and their structures were determined by single crystal X-ray crystallographic and spectrochemical methods.The complex (1) and (2) consist of 1D polymeric chains by bridging of btc2-_ ligand into macrocyclic complexes.in crystalline solids. Interaction of Cu-O9 (2.498 Å), Cu-O14 (2.496 Å) and Ni-O5 (2.859 Å), Ni-O9 (2.825 Å) formed 1-D chain structures in crystalline 1 and 2, respectively.



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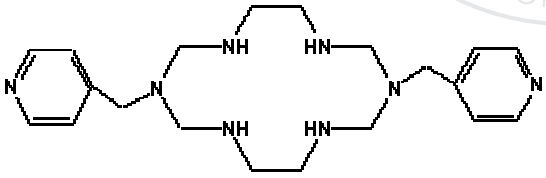
Preparation and structure of supramolecules obtained by the combination of cyclic polyazamacrocyclic complexes and tetracyanometallate.

엔크줄, 곽지훈

순천대 화학과

The synthesis of crystal structures by design is a key objective for modern chemistry. Usually, supramolecular structures of complexes are achieved by self-assembly using directional intermolecular interactions implemented in supramolecular building blocks. Here, we synthesized the complexes by combination of [M(L)]2+ (where, M = Ni(II) and Cu(II)) and [MX4]2-(where M=Pt, Ni, X=CN). The copper(II) and Ni(II) macrocyclic complexes produced 1-D and 2-D chain in crystalline solids. The design, construction and x-ray structure of obtained supramolecular systems are discussed in detail.



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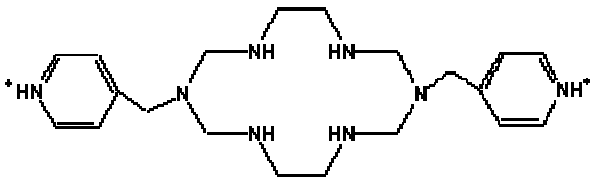
Design and construction of supramolecules obtained by the combination of protonated cyclic polyazamacrocyclic complexes and square-planar anionic complexes.

엔크줄, 곽지훈

순천대 화학과

The combination of coordination and hydrogen bonding in supramolecular architecture has provided particularly interesting supramolecular systems with unique topologies and potentially useful properties. Here we used polyazamacrocyclic complexes of nickel(II) and copper(II), [M(H2L)]4+, where L = 1,8-bis(4-methylpyridyl)-1,3,6,8,10,13-hexaazacyclotetradecane, in which two proton donor groups are attached to the pyridyl nitrogen atoms on side chains as cationic building blocks and a square planar complex of [MX4]2-. Where M = Ni or Cu and X = CN- or Cl-, and X2 = dto. In this presentation, the strategic design, construction and x-ray structure of self-assembled networks combined these macrocyclic complexes and appropriate square planar complexes will be discussed in detail.



H_2L

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Synthesis and reactivities of Pd(0) complexes containing NHC (N-heterocyclic carbene) ligand

김용주, 이정현, *이경은, *이순원

*강릉대 화학과 *성균관대 화학과*

Zerovalent Pd compounds having NHC carbene ligands (IPR = 1,3-bis(2,6-diisopropylphenyl)imidazol-2-ylidene or SIPr = 1,3-bis(2,6-diisopropylphenyl)-4,5-dihydroimidazol-2-ylidene) were prepared from reactions of Pd(styrene)L2 with IPR or SIPr. Oxidative addition of organic halides toward the zerovalent Pd compounds afforded corresponding new Pd compounds via C-Cl or C-Br cleavage. Interestingly, the unique oxidative addition of dichloromethane as a solvent toward the zerovalent Pd compounds was observed.

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Synthesis and structures of tetrazole-thiolato Pd(II) and-Pt(II) complexes

김용주, 이혁희, 한삼용, 경영수, *이경은, *이순원

*강릉대 화학과 *성균관대 화학과*

Reactions of bis(azido)Pd(II) or -Pt(II) complexes with chiral isothiocyanates(R-NCS) gave various tetrazole-thiolato Pd(II) and -Pt(II) complexes. X-ray structural analyses on the isolated compounds shows selective formation of chiral tetrazole-thiolato compounds depending on the isothiocyanates as substrates. Experimental details will be discussed.

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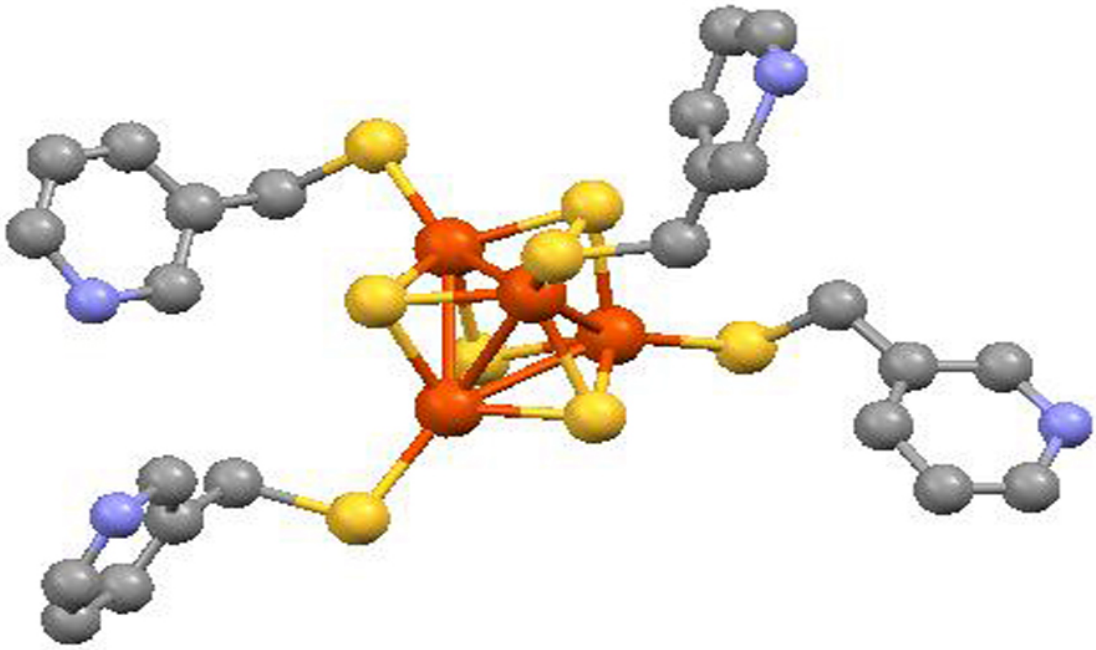
Synthesis and Characterization of Fe/S Clusters with 2-,3-, and 4-Pyridinemethanethiolate Terminal Ligands

김유진, 한재홍

중앙대 생명공학과

As new iron sulfur cluster ligands, 2-, 3-, and 4-pyridinemethanethiol were synthesized from 2-, 3-, and 4-picolyl chloride hydrochloride, respectively, with thiourea in dH_2O under N_2 atmosphere. 4Fe-4S and 2Fe-2S clusters were synthesized in acetonitrile and tetrahydrofuran, respectively, according to the published methods and identified by IR, UV-VIS spectroscopy, and elemental analysis. Each ligand was reacted with clusters using co-solvent system under N_2 atmosphere. All the new Fe/S clusters were characterized by IR, UV-VIS, and CV. Structures of complexes were determined by single crystal X-ray crystallography.



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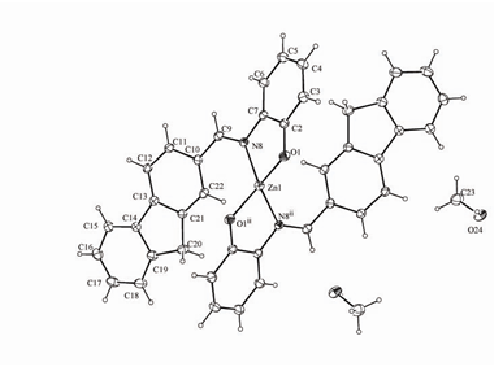
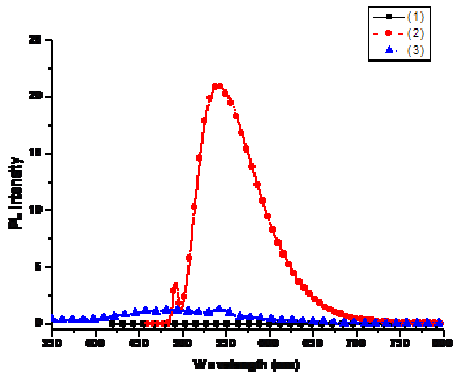
Luminenscence Zn(Ⅱ) Complexes Based on N^O, N^N^O and N^N^N Schiff Bases

송영광, *서희주, *윤성재, **김영인

*부산대 첨단정보 및 디스플레이소재협동과정 *부산대 화학과 **부산대 화학교육과*

We prepared new luminescent Zn(Ⅱ) complexes by the reaction of zinc acetate with (E)-2-((9H-fluoren-7-yl)methyleneamino)phenol (L1), 2-((E)-(benzothiazol-2-ylimino)methyl)phenol (L2), and (E)-N-(pyridine-2-ylmethylene)benzothiazol-2-amine (L3) as the light-emitting ligands ; $Zn(L1)_2$ (1), $Zn(L2)_2$ (2) and $Zn(L3)_2$ (3). The emission maxima for the three complexes (1, 2, 3) in DMF solution are at λ=611, 541 and 490 nm, respectively. The luminescence of the complexes are believed to originate from intra-ligand charge transitions ($\pi^* \rightarrow \pi$) of the prepared ligands. The HOMO and LUMO energy levels were calculated from the electrochemical and optical properties. The complex 1 was structurally characterized using single crystal X-ray method. The Zn atom adopts a tetrahedral geometry, being ligated by two N atoms and two O atoms in L1 ligand.





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Preparation of New mixed-ligand Titanium(Ⅳ) guanidinate Complexes for Titanium Precursors.

정인경, 김창균, 정택모

한국화학연구원 화학소재연구단

Titanium-containing precursors find a variety of applications in microelectronics for the deposition of pure metal, nitride, and oxide. As a metal, titanium is used as a metal electrode, but due to its high tendency toward oxidation, titaniumnitride is typically deposited as a capping layer. The most important applications for titaniumnitride are employment as an N-type gate metal and as a metal electrode invarious capacitor applications. In addition, thin films of TiN have been used in solar cells, as hard and decorative coatings, and in optics. There is an increasing interest in titanium oxide due to its high k value. It can be deposited either as the pure oxide or with other oxides. For instance, with strontium oxide, it will formthe ultra-high-k ternarymaterial SrTiO3, with a k value that may exceed 300.We introduce a new class of volatile and thermally stable titanium precursors.Novel Titanium(Ⅳ) guanidinate Complexes were synthesized by the reaction of titanium compounds with guanidinate ligands. New Titanium(Ⅳ) guanidinate Complexes have been characterized by NMR, FT-IR, mass spectroscopy, and elemental analysis. Thermal analysis has also been performed to qualitatively evaluate their volatility.

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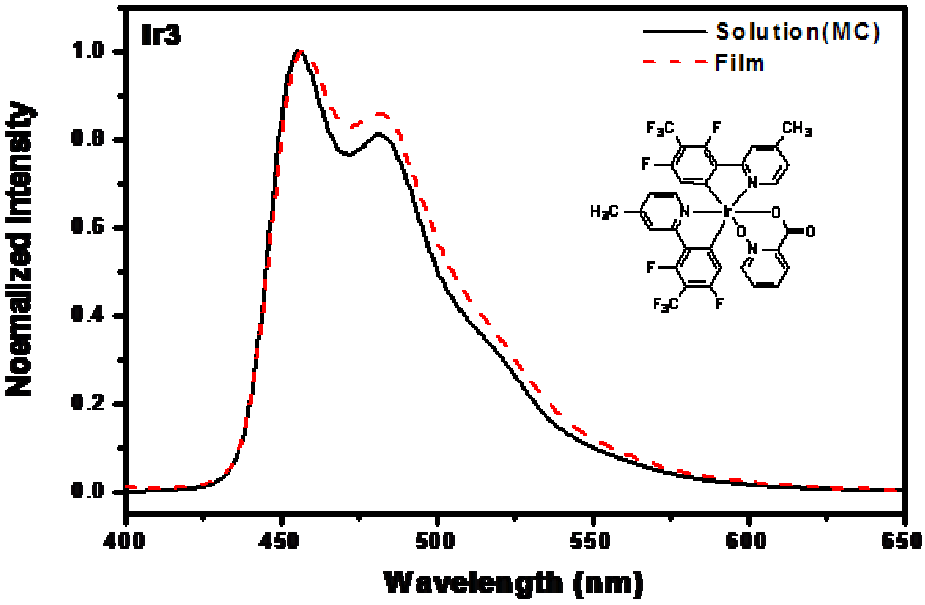
발표분야: 무기화학
발표종류: 포스터, 발표일시: 목 10:30~12:30

Synthesis and Characterization of New Blue Phosphorescent Ir(III) Complexes for High Efficiency Organic Light-Emitting Diodes (OLEDs)

서회주, 윤성재, *송영광, **진성호, **김영인

*부산대 화학과 *부산대 첨단정보 및 디스플레이소재협동과정 **부산대 화학교육과*

Organic light-emitting diodes (OLEDs) have gained many interest in blue phosphorescent Ir(III) complexes with high efficiency and deep-blue color. We synthesized blue phosphorescent Ir(III) complexes, (F_2CH_3ppy)Ir(picN-O) (1), (F_2CH_3ppy)Ir(ppc) (2), ($F_2CF_3CH_3$ppy)Ir(picN-O) (3) and ($F_2CF_3CH_3$ppy)Ir(ppc) (4), for applications in OLEDs. The Ir(III) complexes have high phosphorescent quantum yields as well as high thermal stability. High performance OLEDs fabricated using 1 and 3 showed blue emission with the CIE coordinates of (0.161, 0.278) and (0.149, 0.193) at the current density of 0.1 mA/cm^2, and high external quantum efficiencies of 19.6 and 21.4 %.



대한화학회
THE KOREAN CHEMICAL SOCIETY

일시: 2010년 4월 29~30일(목~금) 2일간
장소: 송도컨벤시아
발표코드: **Ⅰ33P68포**
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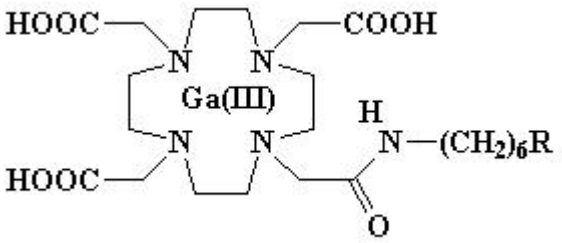
발표종류: 포스터, 발표일시: 목 10:30~12:30

DOTA 유도체의 합성 및 Ga-DOTA 착 화합물의 합성

이홍래, 최상무, 김상욱, 양승대

한국원자력연구원 방사선생명공학연구부

현재 국내외에서는 $^{68}Ge/^{68}Ga$ 방사선발생장치를 이용하여 ^{68}Ga 을 도입한 방사성의약품으로 연구 및 개발이 진행되고 있다. 이번 연구는 DOTA 유도체 및 Ga-DOTA 착 화합물을 합성하고 HPLC 로 분리하고, NMR 과 같은 분광기를 이용하여 확인하였다. DOTA 유도체는 카르복실기 중 하나에 아미드 결합을 통한 연결고리를 늘렸다. 합성된 DOTA 유도체와 Ga 과의 배위를 진행하였다. DOTA 유도체의 합성수율은 20-30%이었으며, Ga-DOTA 착 화합물의 합성수율은 약 40%이었음을 확인하였다.



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발표코드: **Ⅰ33P69포**
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발표종류: 포스터, 발표일시: 목 10:30~12:30

Novel Germanium Complexes as Promising Precursors for $Ge_2Sb_2Te_5$ (GST)

이유경, *정택모, *김창균

*한국화학연구원 소자재료연구실 *한국화학연구원 화학소재연구단*

The germanium complexes have been synthesized and extensively researched because of their potential applications as precursors for the next-generation, nonvolatile, fast reversible switching and high endurance phase change random access memory (PRAM) based on $Ge_2Sb_2Te_5$ (GST). However some germanium(IV) precursors for MOCVD of Ge alloy films, have the defects of high deposition temperatures, low vapor pressure in spite of a relatively low deposition temperature, premature decomposition experienced when germane is present. In the present work, we synthesized new Ge complexes as potential sources for MOCVD processes and characterized by means of ^{1}H and ^{13}C NMR, infrared spectra.

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발표종류: 포스터, 발표일시: 목 10:30~12:30

A Facile C-C Bond Cleavage in Acetylacetone by Metalloporphyrin

Atul Pratap Singh, 박부배, 김희준

금오공과대 응용화학과

The C-C bond cleavage is one of the most critical and prominent area of research for long time due its significant use in in-vivo and in-vitro reactions in the synthesis of biologically active organic compounds as well as in the decomposition of environmentally hazardous xenobiotic compounds. Till date very few examples are known in the literature on the C-C bond cleavage where most of them are mainly based on the enzymatic fission. The Fe(II) dependent NHMCD, Acinatobacter johnsonii acetyacetone dioxygenase (Dke1) is representative example to cleave the C-C bonds in β-carbonyl compounds capable of undergoing enolization to a cis-β-keto-enol structure. In this order, we herein present the use of metalloporphyrin for the C-C bond cleavage in β-diketones.

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발표종류: 포스터, 발표일시: 목 10:30~12:30

Crystallographic, optical, and reactivity manifestations of the "8-heteroaryl effect" in N,N-difluoroboryl-5-(Ar)dipyrrin (BODIPY) systems

김기봉, **D.G.Churchill**

KAIST 화학과

In this presentation, N,N-difluoroboryl-5-(*Ar*)dipyrrin (*Ar* = 2-furyl, 7; 2-selenenyl, 9; 3-furyl, 10) have been prepared for comparison to the previously reported thienyl versions (*Ar* = 2-thienyl, 8; 3-thienyl, 11) and were fully characterized by NMR spectroscopy, single-crystal X-ray diffraction, mass spectrometry, elemental analysis, and UV-vis spectroscopy. These species were studied both in the solid state and in solution: subtle structural differences in the crystalline state allow for insights into crystal engineering, whereas solution results show interesting platforms for potential fluorescence bioapplications (e.g., neuro-probing studies). For the 2-heteroatom substitution, Ar species increase in E weight correlates with increasing (i) cell volume and (ii) dihedral angle between the Ar ring and BODIPY core. In absorption and emission spectra, 2-heterocyclic species show higher wavelengths than 3-heterocyclic ones, pointing to an electron withdrawing effect. Increasing E weight gives a lower ϕ_F value. These compounds are quite resistant to decomposition as tested by hydrogen peroxide, but do respond uniformly upon harsh bromination (Br_2).

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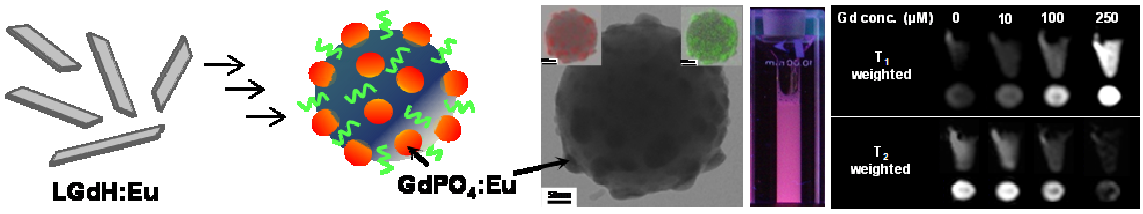
발표분야: 무기화학
발표종류: 포스터, 발표일시: 목 10:30~12:30

Fabrication of a Silica Sphere with Fluorescence and Magnetic Relaxation Properties by Employing the Transformation of Gadolinium Hydroxide Layers into Gadolinium Phosphate Nanoparticles

윤영수, 이인수

경희대 응용화학과

A novel method for modifying the surface of MR contrasting layered gadolinium hydroxide (LGdH) layers was developed to provide them with water- and bio-compatibility and acid-resistance, which are essential for medical applications. A stable colloid of exfoliated layers was synthesized by exchanging interlayer anions of LGdH with oleate ions. The delaminated layers were successively coated with phospholipids with poly(ethylene glycol) tail groups and their effectiveness as a contrast agent for MR imaging was demonstrated. The adaptability of this surface modification approach for incorporating functional molecules and fabricating a fluorescent colloid of LGdH, which has the potential utility as a multimodal probe, was also demonstrated. It is believed that this result will provide a novel approach for expanding the applications of layered inorganic materials and developing a new class of MRI contrast agents.



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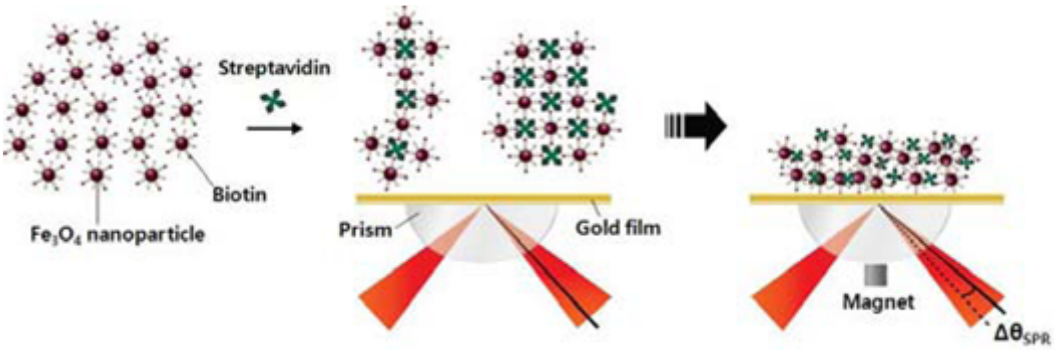
발표종류: 포스터, 발표일시: 목 10:30~12:30

Novel Surface Plasmon Resonance Detection Based on Superparamagnetic Nanoparticles and External Magnetic Fields

이경식, 박봉현, 이인수

경희대 응용화학과

In this study, novel surface plasmon resonance (SPR) detection based on superparamagnetic iron oxide nanoparticles (SPIONs) and external magnetic fields was demonstrated. Aggregates of streptavidin (SA) molecules bound with biotinylated SPIONs were attracted adjacent to a metal film and created a layer with a refractive index contrast only when magnetic fields were externally applied, resulting in a notable SPR angle change. The experimental results indicated that the concentrations of the reactants such as SA and the size of the SPIONs play important roles in achieving enhanced SPR sensing. As a result, this study illustrates the potential for sensitive and selective detection of target molecules without the requirement of immobilized receptors on the sensor surface.



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Metallotubulanes Consisted of Ag(I) and Calix[4]arene Spacers

박기민, 김현지, 박인혁, 이심성

경상대 화학과

In order to develope supramolecular coordination polymers, we have designed and synthesized the potassium salt of calix[4]arene tetracarboxylate ($CTCK_4$, $\{[K_2(K_2@CTC)(H_2O)_7\}_n$) and calix[4]arene tetrabenzoate ($CTBK_4$) with 1,3-alternative conformation. Self-assembly of $CTCK_4$ and $CTBK_4$ with Ag(I) ion affords to metallotubulane $CTCAg_4$ ($\{[Ag_2(Ag_2@CTC)]\bullet 4H_2O\}>\}_n$) and $CTBAg_4$ $\{[Ag_4(CTB)(H_2O)(CH_3OH)_3](H_2O)_2\}_{n/}$), respectively. In the crystal structures of both metallotubulanes, the number of Ag(I) ion linking calix[4]arene spacers is different from each other. In $CTCAg_4$, four carboxylates of CTC are coordinated to four Ag(I) ions. However four carboxylates of CTB in $CTBAg_4$ are coordinated to eight Ag(I) ions due to the conjugation of negative charge of carboxylate with aromatic electrons. In additionally, it is interesting that two potassium ions captured inside both interstitial cavities of CTC were substituted by two silver ions in the process of the self-assembly of $CTCAg_4$. This substitution of cations in solution state is explored by ^{1}H-NMR titration.

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발표종류: 포스터, 발표일시: 목 10:30~12:30

Extraordinary stable ammonium ion complex of a noncyclic crown-type polyether: solid and solution studies

박기민, 김현지, 정종화, *Jagadese J. Vittal, 이심성

*경상대 화학과 *National University of Singapore*

Among the noncyclic crown-type polyethers, 1,13-bis(8-quinolyl)-1,4,7,10,13-pentaoxatridecane [L, Kryptofix-5®] is a representative example due to its similar behaviours with 18-crown-6 because it has the attractive capability to form the pseudo-cyclic complexes with cationic guests in a manner similar to cyclic species. In addition, its stoichiometric complexation with ammonium ion has been introduced by Vögtle et al as early as 1977. It is amazing that no crystal structure of its ammonium ion complex is available till now even though the knowledge of such structural information has been a prerequisite for the progress of the recognition of the organic and biomolecules. Therefore, in an extension of our work on complexation of L, we prepared the crystalline complex of L with ammonium ion suitable X-ray analysis. We herein report the preparation and crystal structure of ammonium ion complex of L. The photophysical and thermal properties of the complex are also discussed. In addition to the solid-state study, NMR titrations of L and 18-crown-6 with ammonium ion in acetonitrile were undertaken to compare the stability constants of the complexation.

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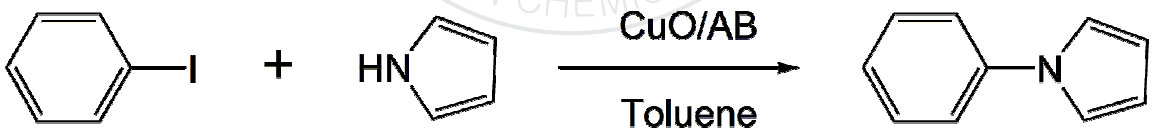
발표분야: 무기화학
발표종류: 포스터, 발표일시: 목 10:30~12:30

Highly Efficient and Reusable Copper-Catalyzed N-Arylation ofNitrogen-Containing Heterocycles with Aryl Halides

배희선, 김아영, *박지찬, 양해식, *송현준, 박강현

*부산대 화학과 *KAIST 화학과*

An environmentally sound process for CuO/AB catalyzed N-arylation has been developed. The CuO/AB was found to be a simple and efficient catalyst for a variety of nitrogen-containing heterocycles with aryl halides. In addition, the CuO/AB was readily separated by centrifugation and could be reused ten times under the present reaction conditions without any loss of catalytic activity. These results confirm that the catalytic system presented herein satisfies the conditions for heterogeneous catalysts of ease of separation, recyclability, and persistence. These heterogeneous systems are promising industrial catalysts with the concept of chemical economy



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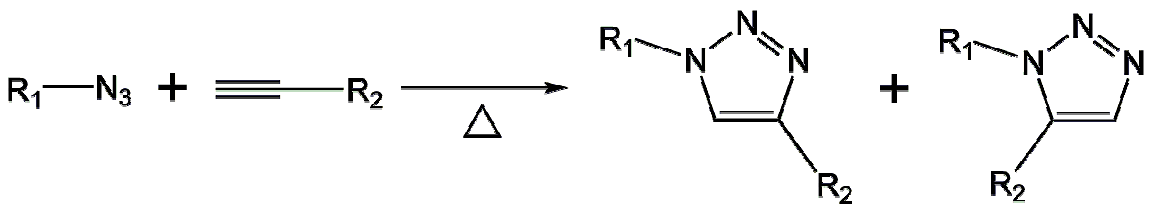
발표종류: 포스터, 발표일시: 목 10:30~12:30

Solvent-Free Microwave Promoted [3+2] Cycloaddition of Alkyne-Azide in Uniform CuO Hollow Nanospheres

김아람, *박지찬, *송현준, 박강현

*부산대 화학과 *KAIST 화학과*

The formation of a triazole-containing carbon-heteroatom bond through Huisen [3+2] cycloadditions is a representative example of a click reaction. The research presented here intends to use immobilized Cu(II) nanoparticles for click chemistry. CuO hollow nanospheres on acetylene black (CuO/AB) have been used for the catalytic [3+2] cycloaddition of azides with terminal alkynes without solvent, and within one minute under microwave irradiation. After the reaction, the CuO on AB was separated by centrifugation and reused five times under the same reaction conditions without any loss of catalytic activity. Thus, as a result of this study, a process of triazoles production has been developed, which is environmentally friendly.



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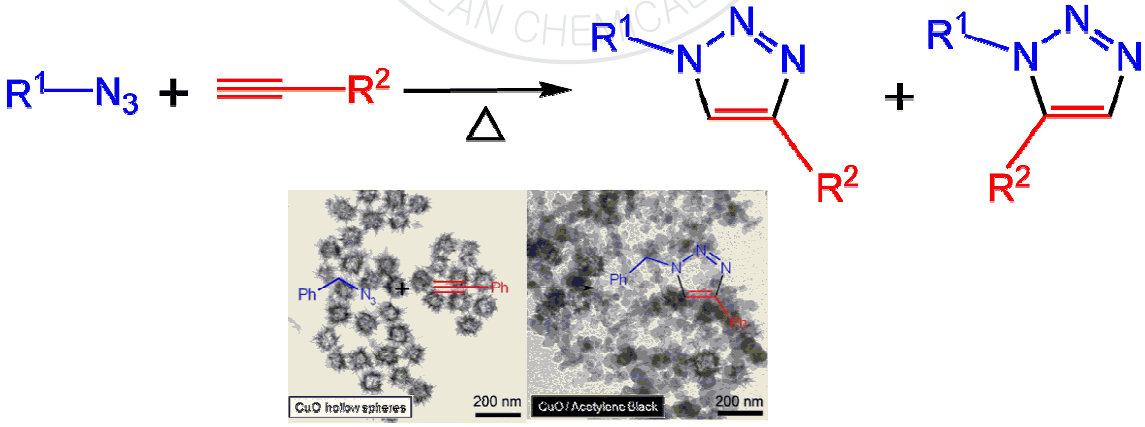
발표종류: 포스터, 발표일시: 목 10:30~12:30

Immobilized CuO Hollow Nanospheres Catalyzed Alkyne-Azide Cycloadditions

허은정, *박지찬, *송현준, 박강현

*부산대 화학과 *KAIST 화학과*

An approach for gram-scale synthesis of uniform Cu_2O nanocubes by a one-pot polyol process was used. The CuO hollow nanostructures were prepared by adding aqueous ammonia solutions with Cu_2O nanocube colloidal solutions. CuO hollow nanospheres on acetylene black (CuO/AB), were synthesized and used for the catalytic [3+2] cycloaddition of azides with terminal alkynes to provide products in good yields with high regioselectivity. The CuO/AB was readily separated by centrifugation and could be reused ten times under the present reaction conditions without any loss of catalytic activity.



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발표종류: 포스터, 발표일시: 목 10:30~12:30

Cobalt(III) Complexes of Various Salen-Type Ligand Bearing Four Quaternary Ammonium Salts and Their Reactivity for CO_2/Epoxide Copolymerization

박은석

아주대 응용화학

Ligand variation on a cobalt(III) complex of Salen-type ligand comprised of 1,2-cyclohexenediamine and salicylaldehyde bearing a methyl substituent on its 3-position and -[$CMe(CH_2CH_2CH_2N^+Bu_3)_2$] on its 5-position, which is a highly active catalyst for CO_2/propylene oxide copolymerization, was carried out. Replacement of the methyl substituent on 3-position with bulky isopropyl group resulted in alteration of the binding mode, consequently lowering TOF significantly. Replacement with ethyl group preserved not only the binding mode but also the activity. Either replacement of tributylammonium unit with trihexylammonium or trioctylammonium or replacement of 1,2-cyclohexenediamino unit with -$NC(Me)_2CH_2N$- decreased the activity even though the binding mode was unaltered.

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Electronic and Optical Characterization of Silafluorene and Its Application as an Expolsive Sensor

양진석, 조성동, 손홍래

조선대 화학과

1,1-dialkyl or diaryl substituted silafluorenes have been synthesized and their electronic and photonic behaviors were investigated. An absorption spectrum of 1,1-dimethyl silafluorene showed its absorption band at 292 nm. They also displayed an emission band at 349 nm with an excitation wavelength of 292 nm in solution. Their emission behaviors were investigated both in the solid state and colloid state. Quantum yield of 1,1-dimethyl silafluorene was measured in solution and colloid. In the solid state, 1,1-dimethyl silafluorene displayed an emission wavelength at 415 nm, indicating that the emission wavelength in the solid state was shifted to the longer wavelength by 66 nm. Characteristics of organic-light emitting diode (O-LED) for the 1,1-dimethyl silafluorene were obtained. The structure of OLED devices was ITO/CuPc/TPD/1,1-dimethylsilafluorene/Alq3/LiF/Al. An electroluminescence spectrum of 1,1-dimethyl silafluorene was obtained from OLED characteristics, indicated quite similar results from solid state emission spectrum, and displayed an emission band at 409 nm, which was shifted to the shorter wavelength by 6 nm. I-V characteristis for the 1,1-dimethylsilafluorene was obtained from the applied voltage versus luminance and current density plot. Its electroluminescence start at 15 V and its maximum luminance was 245 cd/m2 at given conditions. 1,1-Dimethylsilafluorene was served as a chemical sensor. Detection of nitroaromatic compound was achieved by measuring the quanching photoluminescence of 1,1-dimethylsilafluorene. This research was financially supported by the Ministry of Education, Science Technology (MEST) and Korea Institute for Advancement of Technology (KIAT) through the Human Resource Training Project for Regional Innovation.

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발표종류: 포스터, 발표일시: 목 10:30~12:30

Detection of CRP Based on anti-CRP DBR Porous Silicon Interferometer

최태은, 조성동, 손홍래

조선대 화학과

Distributed Bragg reflector (DBR) porous silicon (PSi) exhibiting unique reflectivity was successfully obtained by an electrochemical etching of silicon wafer using square current waveform. A biosensor was described an optical interferometric transducer scheme based on inexpensive and readily available optically flat thin films of DBR PSi. The system was probed with various fragments of an aqueous C-reactive protein (CRP) analyte. The sensor operated by measurement of the reflection peak in the white light reflection spectrum from the porous silicon layer. Molecular binding was detected as a shift in wavelength of reflection peaks. This research was financially supported by the Ministry of Education, Science Technology (MEST) and Korea Institute for Advancement of Technology(KIAT) through the Human Resource Training Project for Regional Innovation

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발표종류: 포스터, 발표일시: 목 10:30~12:30

Versatile Methods for Synthesis of Graphene Sheets from Graphite

진성훈, *조성동, *손홍래

*조선대 화학과 *조선대 화학과*

The unique electronic property of graphene sheets provide potential applications in nanocomposites and fabricating various microelectrical devices, such as field - effect transistors, ultrasensitive sensors, and electomechanical resonators. Several effective techniques have been developed for preparing graphene sheets. Among these technique, mechanical exfoliation can produce pure graphene and epitaxial graphene sheets have been prepared by treatment of silicon carbide wafers at high temperature. Recently, graphene sheet have been developed by chemical reduction method from graphene oxide. in this work, we have synthesized graphene sheets based on mechanical exfoliation and chemical reduction methods. Graphene sheets were characterized by field-effect scanning electron microscope(FE-SEM). The size of graphene sheets was from few hundreds nanometer to decades micrometer. Futher details will be presented. This research was financially supported by the Ministry of Education, Science Technology (MEST) and Korea Institute for Advancement of Technology(KIAT) through the Human Resource Training Project for Regional Innovation

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

조보민, 조성동, 손홍래

조선대 화학과

Porous silicon films were prepared by an electrochemical etch of n-type silicon (phosphorous doped, orientation) in an ethanolic solution of hydrofluoric acid. Photoluminescence of porous silicon was investigated by controlling of an etching time and applied current densities from 50 sec. to 900 sec. and from 50 mA/cm2 to 800 mA/cm2, respectively. Photoluminescence efficiencies of prepared porous silicon samples were measured at given applied current density. As etching time increased, the photoluminescence efficiency of porous silicon prepared increased. However, this photoluminescence efficiency start to decrease, after it reach to the maximum efficiency with further etching time. Porous silicon sample shown the best photoluminescence efficiency was prepared with 200 mA/cm2 of applied current density and with 300 sec of etching time. This photoluminescence of porous silicon was attributed from the quantum confinement of silicon nanocrystals in the porous silicon and used for the detection of nitroaromatic compounds such as TNT (2,4,6-trinitrotoluene), DNT (2,4-dinitrotoluene), and PA (picric acid) in gas phase. Sensing nitroaromatic compounds was achieved from the quanching photoluminescence of silicon nanocrystals. Quenching efficiencies of porous silicon have been measured upon the exposure of analyte-saturated air. The quenching of PL (photoluminescence) is attributed to the electron transfer quenching of quantum-sized nano-crystallites in the porous silicon matrix to analyte. Further details will be presented. -This research was financially supported by the Ministry of Education, Science Technology (MEST) and Korea Institute for Advancement of Technology(KIAT) through the Human Resource Training Project for Regional Innovation.-

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A Simple Route for Fabrication of Sub-30 nm Silicon Nanowire from Block Copolymer Micellar Arrays

방병만, 박수진

울산과학기술대 에너지공학부

블록공중합체와 무전해도금 (Electroless metal deposition)을 이용하여 30 nm 이하의 실리콘 나노와이어를 합성하는 방법에 관한 연구를 수행하였다. 본 연구에서는 실리콘 웨이퍼 위에 이차원적으로 정렬된 구형 마이셀을 얻기 위해 폴리스테렌-블록-폴리비닐피리딘 (PS-b-P2VP)를 자이렌 용매에 녹인 후 스핀코팅하였다. 마이셀 사이에 겹치는 부분을 플라즈마를 이용하여 제거한 후 은을 적당 두께만큼 증착시킨 후 무전해 도금 방법을 이용하여 실리콘을 에칭하였다. 증착된 은 금속은 불산과 과산화수소의 혼합 수용액 상에서 실리콘 웨이퍼 표면에 접촉된 부분과 반응하여 에칭이 발생하며, 실리콘 단결정의 결정면에 따라 에칭의 형태가 달라지게 된다. 실리콘 (100)의 경우 수직으로 에칭이 되고 블록공중합체가 코팅된 부분은 에칭이 되지 않아 블록공중합체 마이셀의 크기를 조절하여 실리콘 나노와이어의 크기를 조절할 수 있다. 위의 합성방법으로부터 간단하고 쉽게 대면적의 균일한 실리콘 나노와이어를 합성할 수 있었다.

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New 1-Naphthalenyl Fluorophores linked to Ferrocenyl Chalcone

전효경, 서우영, 임채미, 이지연, 이수경, 정윤정, 노동윤

서울여대 화학과

Ferrocenyl chalcones with mono- and di-1-naphthalenyl fluorophores were prepared by a base-catalyzed aldol condensation. Two products, Fc-C(O)CH=CH-1Naph (Fc-1Naph) and Fc-(C(O)CH=CH-1Naph)2 (Fc-d1Naph), were spectroscopically characterized. The electrochemical properties investigated by cyclic voltammetry are very similar to those of Fc-2Naph, but the fluorescence properties are entirely different each other: Both compounds show fluorescent spectra (measured in ethanol) centered at λem = 500 nm (λex = 385 nm) and λem = 496 nm (λex = 399 nm), respectively, while that of Fc-2Naph is quenched.

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Electronic and Optical Characterization of Tetraphenyl Germole and Germafluorene

엄성용, 조성동, 손홍래

조선대 화학과

1,1-Dihydro-2,3,4,5-tetraphenylgermole (DHG) and 1,1-Dimethyl-2,3,4,5-tetraphenylgermole (DMG), are synthesized and characterized. Organic light-emitting devices (OLEDs) with the structure of ITO/TPD/DHG/Alq3/LiF/Al have been fabricated and TPD [N,N´-diphenyl-N, N´-bis(3-methylphenyl)-1, 1´-biphenyl-4, 4´-diamine] acts as a hole transporter. Greenish-blue emission at 512 nm is observed, with the maximum luminance of 26.433 cd/m2 at 11 V. The device shows an excellent diode behavior to under the forward bias. 1,1-dialkyl or diaryl substituted germafluorenes have been also synthesized and their electronic and photonic behaviors were investigated. An absorption spectrum of 1,1-dimethyl germafluorene showed sing absorption band. They also displayed an emission band at 350 nm with an excitation wavelength. Their emission behaviors were investigated both in the solid state and colloid state. Quantum yield of 1,1-dimethyl silafluorene was measured in solution and colloid. In the solid state, 1,1-dimethyl silafluorene displayed an emission wavelength shifted to the longer wavelength. Characteristics of organic-light emitting diode (O-LED) for the 1,1-dimethyl silafluorene were obtained. The structure of OLED devices was ITO/CuPc/TPD/1,1-dimethylgermafluorene/Alq_3/LiF/Al. An electroluminescence spectrum of 1,1-dimethyl germafluorene was obtained from OLED characteristics. I-V characteristis for the 1,1-dimethylgermafluorene was obtained from the applied voltage versus luminance and current density plot. 1,1-Dimethylgermafluorene was served as a chemical sensor. Detection of nitroaromatic compound was achieved by measuring the quanching photoluminescence of 1,1-dimethylgermafluorene.
This research was financially supported by the Ministry of Education, Science Technology (MEST) and Korea Institute for Advancement of Technology (KIAT) through the Human Resource Training Project for Regional Innovation.

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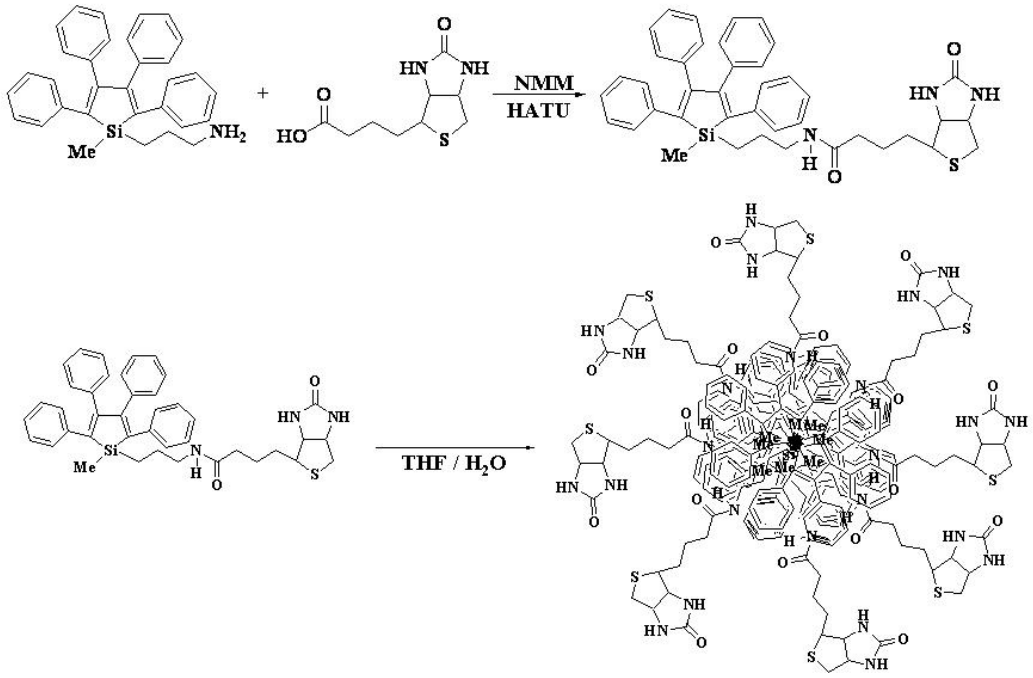
Fluorescence Turn-Off Detection of Biomolecules Based on the Aggregation-induced Emission of Silole

고영대, 조성동, 손홍래

조선대 화학과

By making use of the aggregation-induced emission feature of silole with biotin group is designed synthesis with a view to developing a new optical probe for fluorescence turn-off detection biomlecule. The fluorescence of silole decreases lagely upon mixing with biomolecule, in particular for avidin/streptavin, indicating that silole can be used for fluorescence turn off detection of biomolecule. Here, we report the synthesis of the highly fluorescent siloles derivatized with biotin for searching a possible application as biosensor. Biotin-derivatized silole molecule was obtained from the reaction biotin tetrafluorophenyl ester.-This research was financially supported by the Ministry of Education, Science Technology (MEST) and Korea Institute for Advancement of Technology(KIAT) through the Human Resource Training Project for Regional Innovation.



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Solvent-dependent Fluorescence of 2-Anthracenyl Chalcone

임채미, 이지연, 이수경, 정윤정, 노동윤

서울여대 화학과

Ferrocenyl chalcone with 2-anthracenyl fluorophore, 2Anth-C(O)CH=CH-Fc (2Anth-Fc), was prepared by a base-catalyzed aldol condensation, and spectroscopically characterized. The electrochemical properties investigated by cyclic voltammetry are very similar to those of 9Anth-Fc, but the fluorescence properties are entirely different each other: It shows solvent-dependent fluorescent spectra (λem = 458 nm with λex = 383 nm in chloroform; λem = 448 nm with λex = 378 nm in acetonitrile; λem = 482 nm with λex = 395 nm in ethanol; λem = 489 nm with λex = 392 nm in methanol), while that of 9Anth-Fc is quenched.

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Synthesis and Optical Charactrization of Silole-derivatized Graphene

조현, 조성동, 손홍래

조선대 화학과

Graphite oxide have recently received much attention due to their possible applications in electronic devices, such as field-effect transistors, ultrasensitive sensors, and electromechanical resonators. Siloles have an unusual electronic porperties. These unusual optical and electrical properties can be useful in electronic devices, such as electron transporting materials, light-emitting diodes (LEDs), and chemical sensors. New synthetic routs for silole-derivatized graphene oxide have been developed from the hydrosilylation reaction of 1-methyl-1-aminopropyl-tetraphenylsilole with graphene oxide. Photoluminescence behaviors for the 1-methyl-1-aminopropyl-tetraphenylsilole, graphene oxide, and silole-derivatized graphene oxide were investigated by the measurement of photoluminescence. Prepared graphene oxide and 1-methyl-1-aminopropyl-tetraphenylsilole displayed an emission band at 295 and 480 nm, respectively. Optical behavior of silole-derivatized graphene oxide were investigated by the absorption and fluorescence spectroscopy. The silole-derivatized graphene oxide showed an interesting optical properties. Energy migration by an electron transfer between graphene oxide and silole moiety was observed. The silole-derivatized graphene oxide was further characterized by UV-vis and IR spectroscopy as well as the surface electron micrograph and transmission electron micrograph. Further details for the electronic behaviors of silole-derivatized graphene oxide and reduction to the silole-derivatized graphene will be discussed. -This research was financially supported by the Ministry of Education, Science Technology (MEST) and Korea Institute for Advancement of Technology(KIAT) through the Human Resource Training Project for Regional Innovation

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Development of Synthetic Routes of Silicon Quantum Dots and Their Optical Characterization

김희철, *정현담, *최진규, 손홍래

*조선대 화학과 *전남대 화학과*

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. Recently, in order to utilize the synergetic benefits of Si QDs and quantum dot solids, this laboratory investigated the optical properties of "Si QD solids". There still exist, however, numerous ambiguities regarding this topic, including surface oxidation of Si QD surfaces, electronic communication between QDs, and the extent to which the photoluminescence properties are affected by the synthetic and treatment conditions. 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. - This research was financially supported by the Ministry of Education, Science Technology (MEST) and Korea Institute for Advancement of Technology(KIAT) through the Human Resource Training Project for Regional Innovation.

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Electronic and Optical Characterization of 1,1-Polysilafluorenes and Their Application as an Expolsive Sensor

황민우, 조성동, 손홍래

조선대 화학과

1,1-Dichlorosilafluorenes and 1,1-dihydrosilafluorenes have been synthesized and their electronic and photonic behaviors were investigated. Polycondensation of 1,1-dichlorosilafluorenes and 1,1-dihydrosilafluorenes were conducted by using an Wultz coupling and dehydrocoupling methods, respectively. Absorption and emission spectra for 1,1-dichlorosilafluorenes, 1,1-dihydrosilafluorenes, and 1,1-polysilafluorene were obtained by using UV-Vis and fluorescence spectroscopy in solution, respectively. Their emission behaviors were investigated both in the solid state and colloid state. Quantum yield for 1,1-dichlorosilafluorenes, 1,1-dihydrosilafluorenes, and 1,1-polysilafluorene was measured in solution and colloid, respectively. To compare the detection efficiencies, 1,1-dihydrosilafluorenes and 1,1-polysilafluorene were served as a chemical sensor. Detection efficiency of 1,1-polysilafluorene was much higher compare to that of 1,1-dihydrosilafluorenes, indicating that the delocalization length for 1,1-polysilafluorene was longer than that for 1,1-dihydrosilafluorenes. Detection of nitroaromatic compound was achieved by measuring the quanching photoluminescence of 1,1-polysilafluorene. Other silafluorene derivatives were synthesized and their photonic behaviors were investigated. Further details will be presented. - This research was financially supported by the Ministry of Education, Science Technology (MEST) and Korea Institute for Advancement of Technology (KIAT) through the Human Resource Training Project for Regional Innovation.

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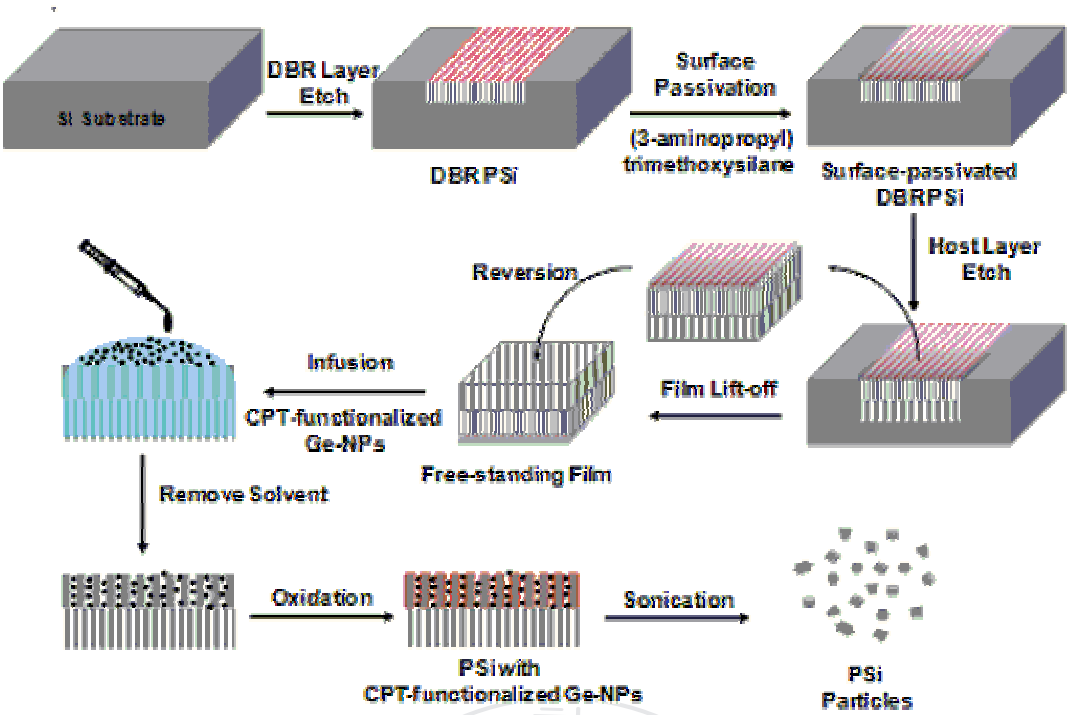
Fabrication and Characterization of PSi Smart Particles Containing 20(S)-Camptothecin-functionalized Germanium Nanoparticle

장승현, 조성동, 손홍래

조선대 화학과

Porous silicon (PSi) smart particles containing 20(S)-Camptothecin (CPT)-functionalized germanium nanoparticles (Ge-NPs) for a noble drug delivery system were developed. PSi samples were prepared by anodization of a highly doped P^{++}-type Si wafer in ethanolic HF solution using a platinum-meshed counter electrode. In this work, PSi was generated by an electrochemical etching of two discrete porous multilayered dielectric mirrors into Si, a top layer was referred to as the “DBR” multilayer, and a bottom layer was the “host” layer intended to infuse CPT-functionalized Ge-NPs. The DBR layer was chemically further passivated with (3-aminopropyl)trimethoxysilane groups. Resulting PSi was removed from the Si substrate by an applying of electropolishing current. CPT-functionalized Ge-NPs were infused into the host layer of PSi free-standing film. Samples were then made into particles by ultrasonic fracture in organic solutions. PSi smart particles were characterized by FE-SEM, FT-IR, EDX, UV-vis absorption, and fluorescence spectroscopy. PSi smart particles containing CPT-functionalized Ge-NPs displayed a linear release profile for the first 12 h, and then perfectly released CPT-functionalized Ge-NPs for 18 h. -
This research was financially supported by the Ministry of Education, Science Technology (MEST) and Korea Institute for Advancement of Technology(KIAT) through the Human Resource Training Project for Regional Innovation



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Detection of Explosives with Fluorescent Thiophene Cavitys Polymer Films.

이보연, 조성동, 손홍래

조선대 화학과

The synthesis, spectroscopy, and fluorescence quenching behavior of pentiptycene-derived phenyleneethynylene polymers. Model cavity thiophene compound containing a pentiptycene bridge have been synthesized to prove detailed structure and spectroscopic insight into conformational effects and electron delocalization. In short, cavity polymer show a larger response to nitro-aromatic compounds, but show a lower response to quinones. Such differences are explained in terms of polymer-analyte interactions, which appear to be electrostatic in nature. The rapid fluorescence response (quenching) of the spin-cast films of porous polymer to nitro-containing compounds qualifies these materials as promising nitroaromtic compounds chemosensor materials.-This research was financially supported by the Ministry of Education, Science Technology (MEST) and Korea Institute for Advancement of Technology(KIAT) through the Human Resource Training Project for Regional Innovation.

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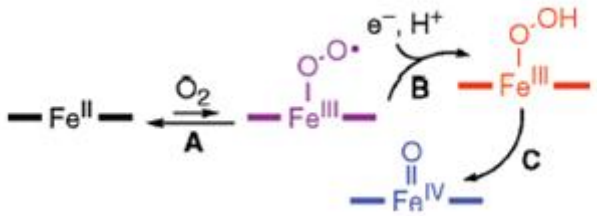
Dioxygen Activation by Mononuclear Nonheme Iron(II) Complexes Generates Iron–Oxygen Intermediates in the Presence of an NADH Analogue and Proton

홍승우, *이용민, **신운섭, ***Shunichi Fukuzumi, ****남원우

*서강대 바이오융합과 *이화여대 기초과학연구소 **서강대 화학과 ***Department of Material and Life Science, Graduate School of Engineering, Osaka University ****이화여대 화학과*

Understanding mechanisms of dioxygen activation of heme and nonheme iron oxygenases is of intense interest in biomimetic research owing to its biological importance and synthetic potential. In this study, we reported the first example of the generation of nonheme iron(III)-hydroperoxo and iron(IV)-oxo intermediates in the presence of dioxygen, proton and NADH analogue. We also have shown that the structure of ligand, spin state and redox potential of iron(II) complex are quite important factors to influence on the feasibility of binding to iron(II) and activating dioxygen.



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Electrochemical Assay of Small Molecules Based on Conformational Changes of Aptamers.

이성은

이화여대 화학 나노과학과

Recently, sensing of small molecules and ions coupling the attractive properties of aptamers has received considerable attention. Electrochemistry offers attarctive routes for interfacing aptamer interactions with the signal generating element in a simple, fast, and inexpensive manner. Modern electronic aptamer biosensors commonly rely on redox tags with conformational changes, or impedance detection to offer convenient measurements of nanomolar concentrations of target molecules. Further enhancement of the sensitivity of such devices is urgently needed for measuring ultra low levels of target agents. Recent studies to improve the sensitivity of aptamer-based biosensors and bioassays have lowered their detection limits to the picomolar level through the use of nanoparticle tags, binding-induced conformational changes, and label-free impedance detection. We herein present an electrochemical aptamer-based sensors with metal complexes as mediators utilizing a specific interaction between DNA and metal complex.

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Fluorescence Detection of DNA Sequences and Potassium Ions Using an Aptamer Probe and a Molecular Light Switch Complex.

오별님

이화여대 화학나노과학과

Convenient fluorescence detection methods for sensing a single base mismatch has been based on the conjugation of a fluorophore at the end of the probe strand or attachment of a fluorophore and a quencher at both ends of the probe DNA. To demonstrate the potential wide applicability of using fluorophores as nucleic acid probes, more simple, label-free sensing systems must be developed. Here, we introduce a new homogeneous assay using rac-Ru(phen)2(dppz)2+ and a K+-binding aptamer for the simple, selective, and sensitive dual assay of a target oligonucleotide and potassium ions depending on how the assay is performed. This method was based on the enhanced emission that occurs when the Ru(dppz) complex interacts with a double-stranded DNA. In addition, the G-quadruplex structure shaped with K+ was disentangled upon the addition of its complementary strand, forming a double-stranded DNA. The target strand detection was selective to other non-complementary oligonucleotides even containing a single base mismatch. In addition, the technique of fast-cooling provides a label-free approach to sensing K+.

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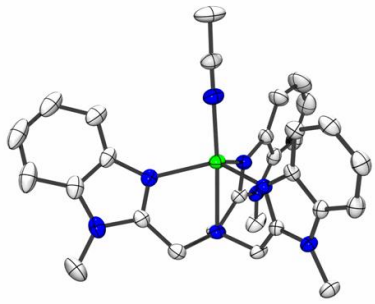
발표코드: **Ⅲ33P41포**
발표분야: 무기화학
발표종류: 포스터, 발표일시: 금 10:30~12:30

A High-spin Oxoiron(Ⅳ) Complex with Tripod Ligand ; Spectroscopy Properties and Reactivites

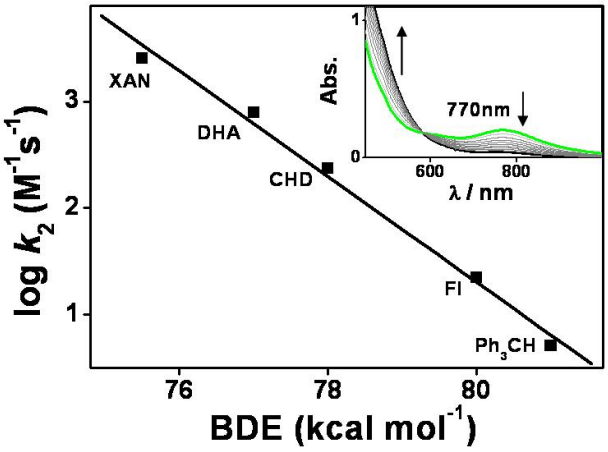
김남희, 서미숙, *남원우

*이화여대 바이오융합과학과 *이화여대 화학과*

High-spin nonheme oxoiron(Ⅳ) species have been frenquently invoked as the reactive intermediates in the catalystic oxidation of organic substrate by mononuclear iron enzymes. Subsequently, we were prepared the Fe(Ⅱ) complex with the tripod ligand,tris(*N*-methylbenzimidazol-2-ylmethyl)amine (Me_3NTB), [$Fe^{II}(Me_3NTB)(CH_3CN)(OTf)_2$], (OTf = trifluromethylsulfonate) and determined as distorted trigonal-bipyramid geometry by X-ray crystallography. The high-spin intermediate was generated by treatment of [$Fe^{II}(Me_3NTB)(CH_3CN)(OTf)_2$] with *m*-CPBA in CH_3CN at -40℃ and extensively characterized with various spectroscopic techniques, including UV-Vis, NMR, EPR, ESI/MS etc. Herein, we report insight into the reactivity of the intermediate with several substrates, such as benzyl alcohol for alcohol oxidation, aliphatic and aromatic alkanes for C-H activation, Ferrocenes for ET etc.



[Fe(Me$_3$NTB)(CH$_3$CN)(OTf)$_2$]



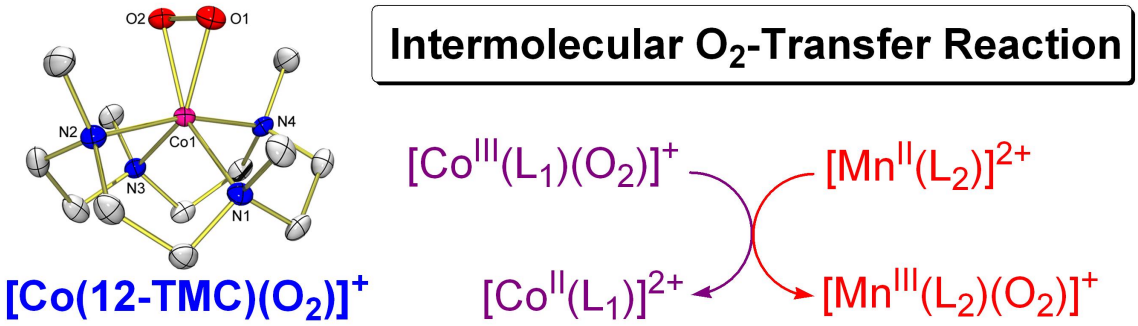
일시: 2010년 4월 29~30일(목~금) 2일간
장소: 송도컨벤시아
발표코드: **Ⅲ33P42포**
발표분야: 무기화학
발표종류: 포스터, 발표일시: 금 10:30~12:30

Mononuclear Cobalt(III)-Peroxo Complexes : Structural andSpectroscopic Characterization and Reactivity in O_2-Transfer

강혜연, 조재홍, 남원우

이화여대 화학나노과학과

Mononuclear metal-dioxygen adducts, M-O_2, are generated as key intermediates in the catalytic cycles of dioxygen activation by metalloenzymes and their model complexes have been characterized, and investigated in electrophilic and nucleophilic reactions. Recently, we reported a crystal structure of a mononuclear side-on nickel(III)-peroxo complex, which shows the O_2-transfer reactivity. Herein, we have shown the synthesis, structural and spectroscopic characterization, and O_2-transfer reactivity of side-on cobalt(III)-peroxo complexes bearing macrocyclic ligands, $[Co(12\text{-}TMC)(O_2)]^+$ and $[Co(13\text{-}TMC)(O_2)]^+$. The reactivity in O_2-transfer reactions is found to depend significantly on the central metal ions and the supporting ligands.



일시: 2010년 4월 29~30일(목~금) 2일간
장소: 송도컨벤시아
발표코드: **Ⅲ33P43포**
발표분야: 무기화학
발표종류: 포스터, 발표일시: 금 10:30~12:30

Reactivity Comparison of Various High-Valent Iron(IV)-Oxo Intermediates

Chen Junying, *홍승우, **이용민, ***남원우

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

High-valent iron(IV)-oxo intermediates have been extensively studied because of their proposed roles in biological and chemical catalysis. To extend our knowledge on biomimetic studies of reactive intermediates, $[Fe^{IV}(O)(TBC)(NCCH_3)_2]^{2+}$ complex (TBC=1,4,8,11-tetrabenzyl-1,4,8,11-tetra-azacyclotetradecane) was generated by PhIO and characterized by various spectroscopic methods. Surprisingly, reactivity of $[Fe^{IV}(O)(TBC)(NCCH)_3]^{2+}$ is much greater, by factor of 2 order, than that of $[Fe^{IV}(O)(TMC)(NCCH)_3]^{2+}$ reported, in which four benzyl groups of TBC ligand has been substituted by methyl groups. We have also shown the reactivity comparison of various iron(IV)-oxo intermediates.

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발표분야: 무기화학
발표종류: 포스터, 발표일시: 금 10:30~12:30

Acid-Base Effects on High-Valent Iron Porphyrins

박선경, *김선희, **남원우

*이화여대 화학나노과학과 *이화여대 기초과학연구소 **이화여대 화학과*

High-valent iron(IV)-oxo porphyrins have been thought to be the key oxidants in the catalytic cycle of heme-containing enzymes. In particular, iron(Ⅳ)-oxo porphyrin π-cation radical intermediates [$(porp)^{+}Fe^{Ⅳ}$=O], referred to as compound I, are generated via O-O bond cleavage in the reactions of iron porphyrin complex with *m*-CPBA. While the mechanistic studies of O-O bond cleavage have been well accomplished, the mechanism of the reverse reaction, O-O bond formation remains to be answered. Thus, we aim to investigate how oxygen-oxygen bond is formed. In this present work, we have studied the acid-base effects on these high-valent iron porphyrin complexes to model dioxygen bond formation. We found that a new species was generated upon adding base to compound I, which was in turn produced by the addition of acid to this new species. Also this reversible cycle could be repeated several times. The characterization and reactivity study of this new species will be presented.

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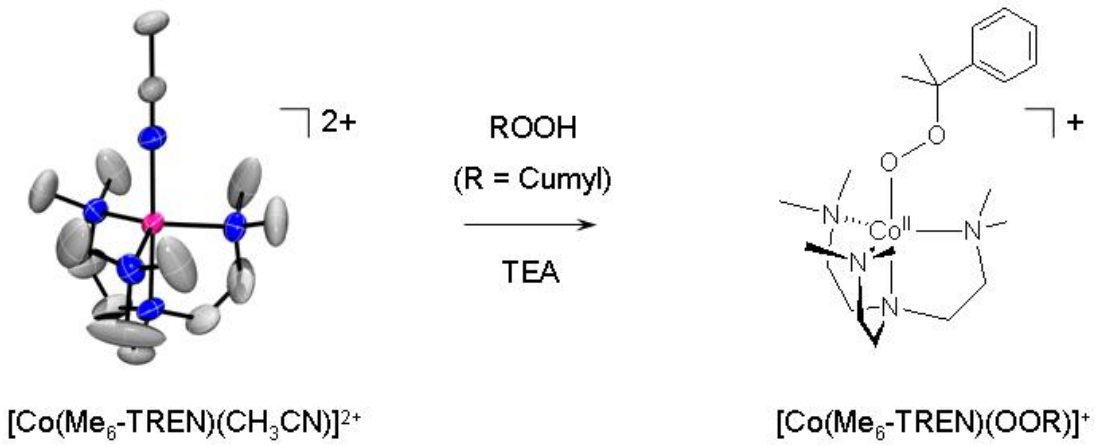
발표분야: 무기화학
발표종류: 포스터, 발표일시: 금 10:30~12:30

Synthesis and Characterization of a High-Spin Co(II)-Alkylperoxo Complex

소정은, *조재홍, **남원우

*이화여대 화학나노과학과 *이화여대 나노과학부 **이화여대 화학과*

Oxidation reactions mediated by metal-alkylperoxo complexes have attracted much attention in the field of bioinorganic and biological chemistry, since the metal-alkylperoxo species are believed to play key roles in the transformation of organic substrates. Recently, reactivity on Co(III)-alkylperoxo complexes has extensively studies in the oxidation of hydrocarbons. Herein, we describe the synthesis and characterization of a high-spin Co(II)-alkylperoxo complex, $[Co(Me_6\text{-TREN})(OOR)]^+$ (R = Cumyl; Me_6-TREN = tris(2-dimethylaminoethyl)amine), which shows reactivity in the oxidation of PPh_3 and CO_2, the latter leading to a μ-carbonato dicobalt(II) complex.



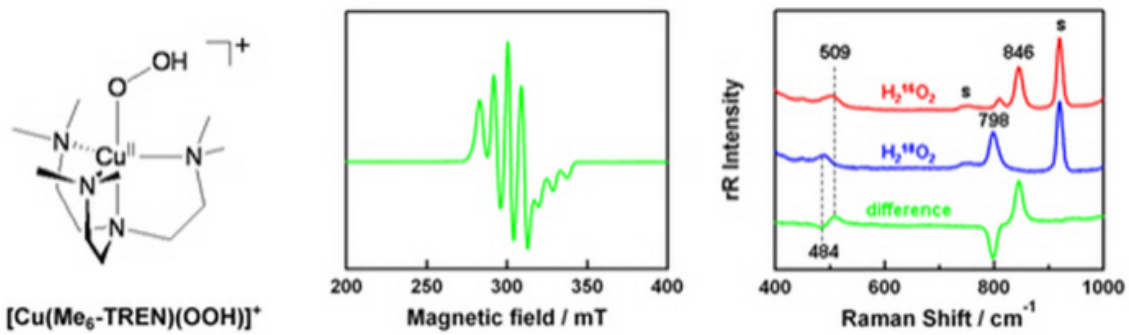
일시: 2010년 4월 29~30일(목~금) 2일간
장소: 송도컨벤시아
발표코드: **Ⅲ33P46포**
발표분야: 무기화학
발표종류: 포스터, 발표일시: 금 10:30~12:30

Characterization and Reactivity of Copper(Ⅱ)-Hydroperoxo Complex Bearing Me_6-TREN Ligand

최유진, *조재홍, **남원우

*이화여대 화학 나노과학과 *이화여대 나노과학부 **이화여대 화학과*

Mononuclear copper centers at the active sites in the metalloenzymes play important roles in O_2 binding, activation, and the hydroxylation for organic substrates. In earlier studies, Cu(II)-hydroperoxo species were proposed to cleave the C-H bond of substrates in enzymatic and synthetic systems. Herein, we report that a Cu(II)-hydroperoxo complex bearing a tetradentate ligand, Me_6-TREN (tris(2-dimethylaminoethyl)amine), was generated in the reaction of $[Cu(Me_6\text{-TREN})]^{2+}$ and H_2O_2 in the presence of base. The intermediate was characterized with various spectroscopic techniques including EPR and rRaman, and investigated in electrophilic and nucleophilic reaction.



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장소: 송도컨벤시아
발표코드: **Ⅲ33P47포**
발표분야: 무기화학
발표종류: 포스터, 발표일시: 금 10:30~12:30

Synthesis, Characterization, and Reactivity Study of a Nonheme Mn(IV)-Oxo Complex

WU XIUJUAN, *Sarvesh C. Sawant, **조재홍, ***서미숙, ****이용민, *****남원우

*이화여대 화학나노과학과 *Department of chemistry Goa University - Goa India **이화여대 나노과학부 ***이화여대 바이오융합과 ****이화여대 기초과학연구소 *****이화여대 화학과*

High-valent manganese-oxo species are frequently been invoked as the important intermediates in the catalytic oxidation of organic substrates by heme and nonheme manganese catalysts. In this presentation, we report the first example of the generation of a mononuclear nonheme manganese(IV)-oxo complex using water as an oxygen source and cerium(IV) as an one-electron oxidant and the spectroscopic characterization, which was performed by EPR, ESI-MS and resonance Raman, and DFT-optimized structure of the intermediate. The source of the oxygen in the Mn(IV)-oxo intermediate was assigned unambiguously by carring out isotopically labeled water experiment. The reactivity of the nonheme Mn(IV)-oxo complex in oxygenation reactions was also discussed.

일시: 2010년 4월 29~30일(목~금) 2일간
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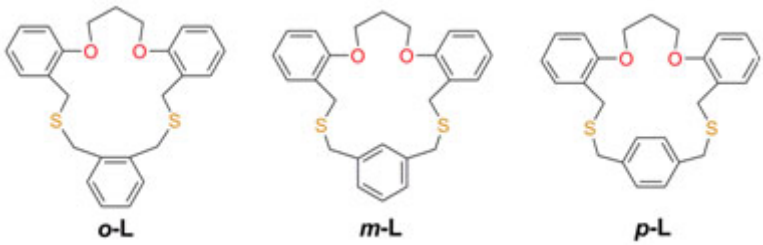
발표분야: 무기화학
발표종류: 포스터, 발표일시: 금 10:30~12:30

Networking of Tribenzo-O2S2-Macrocycles with Mercury(II) Salts: Effect of Macrocyclic Isomers

김현지, 이은지, 이심성

경상대 화학과

Tribenzo-O_2S_2-macrocyclic isomers incorporating a xylyl group in ortho (*o*-L), meta (*m*-L), and para (*p*-L) positions were employed to examine the effect of ligand isomers on supramolecular networking system. In case of mercury(II) thiocyanate, *o*-L and *p*-L afforded infinite 1-D linear (1) and zigzag (2) coordination polymer networks, respectively. But *m*-L gave 2-D square grid type network (3). Notably, the resulting polymeric structures are strongly influenced by the end-to-end bridging of the thiocyanate ion. On the other hand, reactions of mercury(II) halides (Br and I) with *m*-L gave helical type and rhomboid-type 1-D polymers, respectively. In addition, reactions of *p*-L with mercury(II) halides (Cl, Br and I) commonly afforded zigzag 1-D polymers, $[Hg(p\text{-L})X_2]_n$.



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장소: 송도컨벤시아
발표코드: **Ⅲ33P49포**
발표분야: 무기화학
발표종류: 포스터, 발표일시: 금 10:30~12:30

Synthesis and Characterization of Picolinic Tb(III) Compounds

이태우, 강성권

충남대 화학과

[Tb2(3-mePic)7(H2O)][Tb(3-mePic)2(H2O)4]·8H2O was characterized by X-ray single crystal studies and photoluminescence spectraum. Each Tb(III) metal is coordinated to eight atoms (both O and N atoms) to form the distorted square antiprism and the other geometries. We will also discuss the crystal structural features, emission and excitation spectra studies of other Tb(III) compounds.

THE KOREAN CHEMICAL SOCIETY

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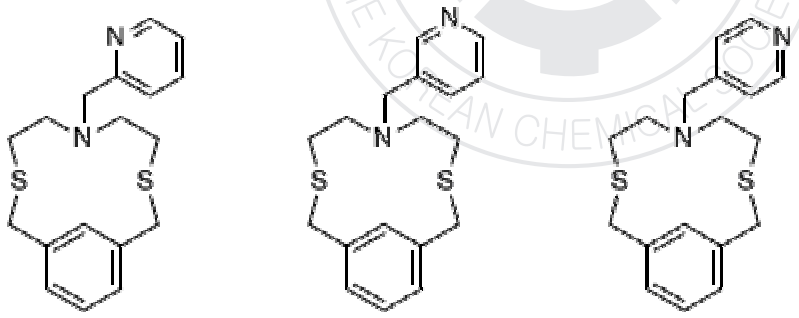
발표코드: **Ⅲ33P50포**
발표분야: 무기화학
발표종류: 포스터, 발표일시: 금 10:30~12:30

NS_2-Donor Macrocycles with Pyridine Arm: Synthesis and Crystal Structures of Ligands and their Supramolecular Soft Metal Complexes

장효정, 박선홍, 이심성

경상대 화학과

NS_2-donor macrocyclic isomer incorporation pyridine pendant in ortho (L^1), meta (L^2), and para (L^3) positions were synthesized to examine the effect of ligand isomers on supramolecular assembly with soft metal self system. Crystal structures of their soft metal complexes with Hg(II) and Ag(I) were prepared and structurally characterized by X-ray crystallography.



L^1 L^2 L^3

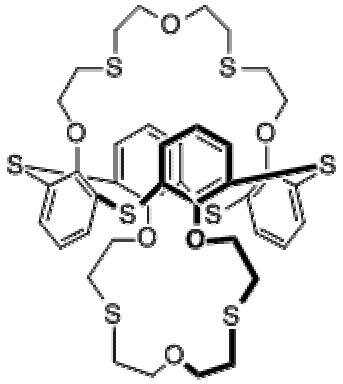
일시: 2010년 4월 29~30일(목~금) 2일간
장소: 송도컨벤시아
발표코드: **Ⅲ33P51포**
발표분야: 무기화학
발표종류: 포스터, 발표일시: 금 10:30~12:30

Anion-Directed Supramolecular Chemistry of An 1,3-alt-Thiacalix[4]arene with Thiaoxacrown-ring: Silver-Based Networking by Exo-Coordination

박선홍, 이심성

경상대 화학과

Thiacalixarenes are modification of classic calixarenes in which methylene bridges between aromatic rings are substituted by sulfur atoms. Coupling reaction of thiacalix[4]arene ditosylate with 2-Mercaptoethyl ether afforded 1,3-alt-thiacalix[4]arene with thiaoxacrown-ring (L). Self-assembled supramolecular networks (1-D, 2-D, and 3-D) were prepared by the reaction of L with silver salts (NO_3^-, ClO_4^-, $CF_3SO_3^-$, and BF_4^-).



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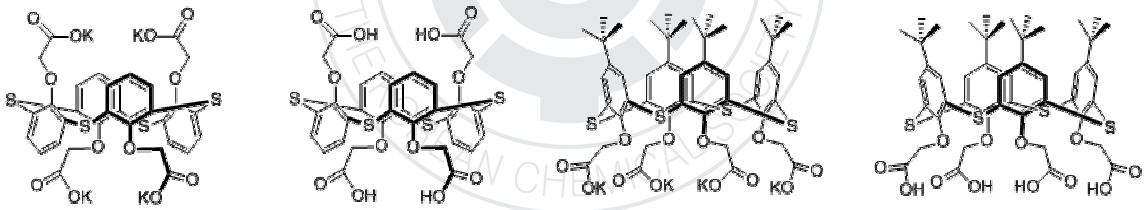
일시: 2010년 4월 29~30일(목~금) 2일간
장소: 송도컨벤시아
발표코드: **Ⅲ33P52포**
발표분야: 무기화학
발표종류: 포스터, 발표일시: 금 10:30~12:30

Synthesis and Complexation of Thiacalix[4]arene Tetracarboxylates

김기환, 박선홍, 이심성

경상대 화학과

Thiacalix[4]arene tetracarboxylates with 1,3-alternate (L^1 and L^2) or cone($L^3$and L^4) conformation were synthesized. Divalent metal complexes of the title receptors (L^1~L^4)with supramolecular structures were prepared and structurally characterized. In complexation, four carboxylic groups act not only as strong dinucleating sites but also as spacer units with cavity.



L^1 L^2 L^3 L^4

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장소: 송도컨벤시아
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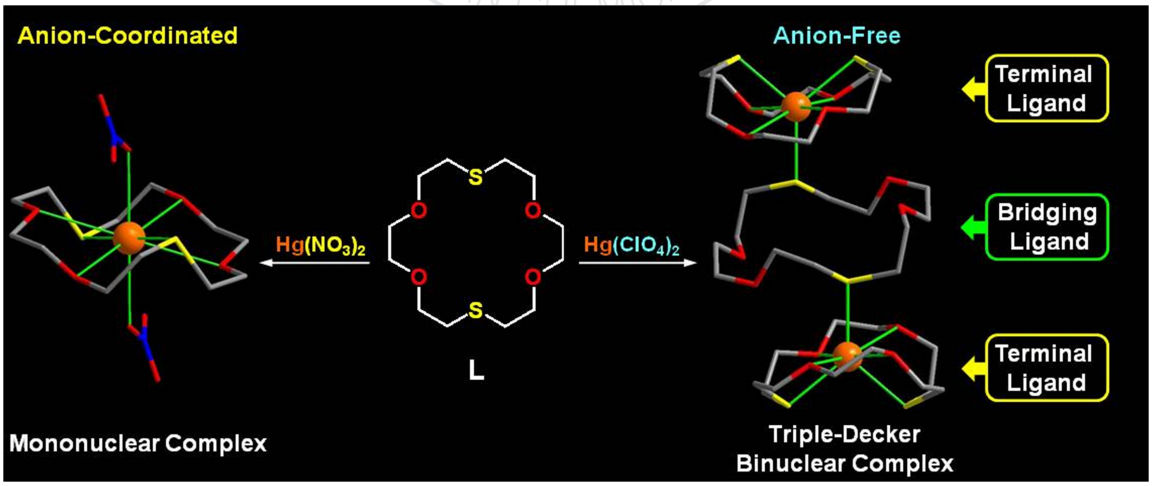
발표분야: 무기화학
발표종류: 포스터, 발표일시: 금 10:30~12:30

New Divalent Metal Ion (M(II) = Ca, Co, Cu, Zn, Cd, Hg, and Pb) Complexes of 1,10-Dithia-18-crown-6: A Revist

박인혁, 박기민, 이심성

경상대 화학과

Since 1,10-Dithia-18-crown-6 (L) was synthesized by R. M. Izatt 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 transition metal ions. Recently, we tried the metallation of L and obtained new 10 complexes (1-10) of L with hard of soft metal ions in benzonitrile. All crystal structures of the complexes were characterized by single-crystal X-ray crystallography. Among the metal complexes of L, $[Hg_2(L)_3](ClO_4)_4$ (7) with 3:2 (L:M) stoichiomerty exhibits very interesting triple-decker type structure see Figure. We will present and discuss about structural characteristics the metal complexes of L.



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발표코드: **Ⅲ33P54포**
발표분야: 무기화학
발표종류: 포스터, 발표일시: 금 10:30~12:30

Basic Research of New Dye for Dye Sensitized Solar Cell

전용우

서경대 응용화학과

Basic Research of New Dye for Dye Sensitized Solar Cell Eun Su Hyeong , Won Mok Jung, Yong Woo Jun and Young Hae Kim Department of Applied Chemistry, Seokyeong University Until now, the dyes for the dye sensitized solar cells (DSSCs) are being used primarily ruthenium complexes and these dyes are regarded as excellent. Among the ruthenium complexes, the red dye N3 and the black dye N749 are the most prominent. But the price for these materials is fairly expensive, thus developing new dyes are necessary for DSSCs. In this lab, we have investigated the absorption and luminescence spectra of the transition - imine complexes for DSSCs. We have been looking for the imine dye whose maximum absorption wavelength (λmax) is observed at near 510nm (red color) and luminescence intensity is much smaller. Λmax of salicylidene-2-aminopyridine was observed to shift to longer wavelength (blue shift) at higher pH (350nm → 410nm at pH 9). Blue shift for the absorption spectra have not been observed when adding several transition metal ions to salicylidene-2-aminopyridine solution (it is not desirable). But transition metal ions made the luminescence intensity decreased considerably. Compared to salicylidene-2-aminopyridine, 2-hydroxy naphthalidene-2-aminopyridine was observed λmax to be shifted to longer wavelength (350nm → 450nm). The absorption spectra change according to pH change and the effect of several transition metal ions are investigated. Solvent: MeOH + H2O (4:1) Fig.1 Structure of 2-Hydroxy-naphthalidene-2-aminopyridine Fig.2 Structure of Salicylidene-2-aminopyridine

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발표분야: 무기화학
발표종류: 포스터, 발표일시: 금 10:30~12:30

Preparation and Structural Characterization of New Cerium(III) Picolinate Complex

오영희, 김장용, 최은주, *이태우, *강성권

*동의대 화학과 *충남대 화학과*

New cerium picolinate complex, $Na_2[Ce(pic)_5]$ · picH · $4H_2O$(pic=picolinate), has been prepared from the reaction of $CeCl_3$ · $7H_2O$ and α-pyridoin anion in methanol solution and structurally characterized by X-ray crystallography. The complex is stable in the air and its crystal structure has been identified as bicapped square antiprismatic geometry with ten coordination.

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발표코드: **Ⅲ33P56포**
발표분야: 무기화학
발표종류: 포스터, 발표일시: 금 10:30~12:30

Oxidation of the Mononuclear Manganese Complex Containing Sterically Hindered Carboxylates

김기역

국민대 화학과

The environmental pollution caused by exhaustion of chemical energy source grows to be global issues. In future, civilization should be sustained using renewable energy from sun without generation of green gases. In recent studies on such renewable energy, many researchers are showing much interest in hydrogen energy generated from solar energy.1) Hydrogen gas has merits to be capable using unlimited capacity and high fuel efficiency. In this context, it is essential to enhance our basic understanding of the fundamental chemical steps involved in such processes. In nature the PSII involves a manganese cluster which acts as an Oxygen-evolving center(OEC). Driven by light energy, from two water molecules, presumably bound to the Mn complex, dioxygen and hydrogen is produced in a five-stepped catalytic cycle. This biologically most important reaction generates the atmospheric oxygen. The molecular mechanisms of such systems, including the extensively studied ruthenium complex (blue dimer) are generally thought to involve metal oxo intermediates and bimolecular steps, but clarification of the fundamental chemical principles responsible for O–O bond formation remains a considerable challenge. With these facts in mind, we focussed on artificial metal oxo complex for mimicking the PSII system.For this reason, we focused and the synthesized mononuclear manganese complex, $Mn(O_2CAr^{Tol})_2(Hdmpz)_2$, where Hdmpz is 3,5-dimethyl pyrazole, has the tetrahedral N_2O_2 coordination environment with two nitrogen atoms from pyrazole ligands and two oxygen atoms from sterically hindered carboxylates. Addition of water molecules to $Mn(O_2CAr^{Tol})_2(Hdmpz)_2$ compound results in water containing $Mn(O_2CAr^{Tol})_2(H_2O)(Hdmpz)_2$ compound. The characterization and reactivity of $Mn(O_2CAr^{Tol})_2(H_2O)(Hdmpz)_2$ including electrochemistry will be presented.Acknowledgement: This work was supported by the Korea Science and Engineering Foundation(KOSEF) grant (NO. R01-2008-000-11812-0) funded by the Korea government(MEST)

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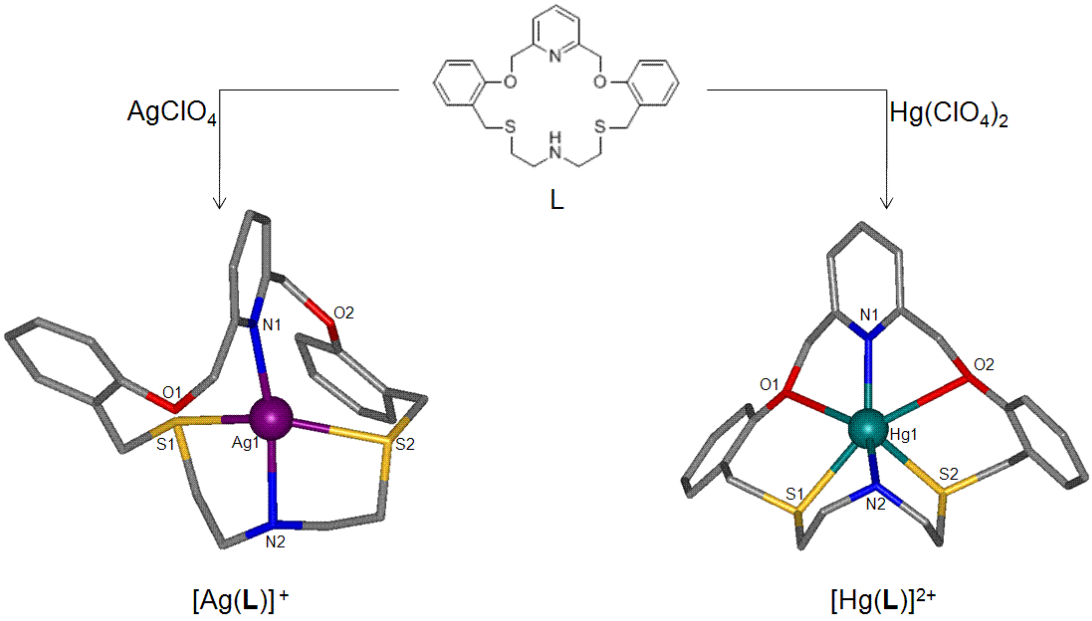
발표분야: 무기화학
발표종류: 포스터, 발표일시: 금 10:30~12:30

Supramolecular Soft Metal Complexes of Thiaoxaaza Macrocycles having Pyridine Subunit

정다람, 이심성

경상대 화학과

The pyridine-containing thiaoxaaza macrocycle L and its complexes with soft metals were synthesized and structurally characterized. L was synthesized from ring closure reaction between corresponding dichloride and dithiol in the presence of Cs_2CO_3 under high dilution condition. L forms endo-type mononuclear complexes with Hg(ll) and Ag(l) via $S_2O_2N_2$-donor atoms.



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Synthesis and characterization of Metal-Cyclam-TTF derivative Complex

이주은, 이홍인

경북대 화학과

Charge-transfer salts, composed of TTF (tetrathiafulvalene) and metal ions, exhibit interesting electric and magnetic properties. We have synthesized Cu(II)/Ni(II) macrocycle-TTF complexes in which the TTF is functionalized with carboxylate groups, BCDT-TTF [Bis(4(5)-carboxy-1,3-dithiolidene)]. BCDT-TTF occupied the axial positions of Ni(II) macrocycle through oxygen atoms to form extended 1-D chain framework. In the case of Cu(II) macrocycle, BCDT-TTF did not form direct coordination to Cu(II). Now we adapt new kind of macrocyclic building blocks, such as metal-cyclam, to synthesize multi-dimensional metal-cyclam-TTF complexes. Metal-cyclam-TTF complexes are characterized by various analytical methods including EA (Elemental Analyzer), EPR (Electron Paramagnetic Resonance), IR, and UV.

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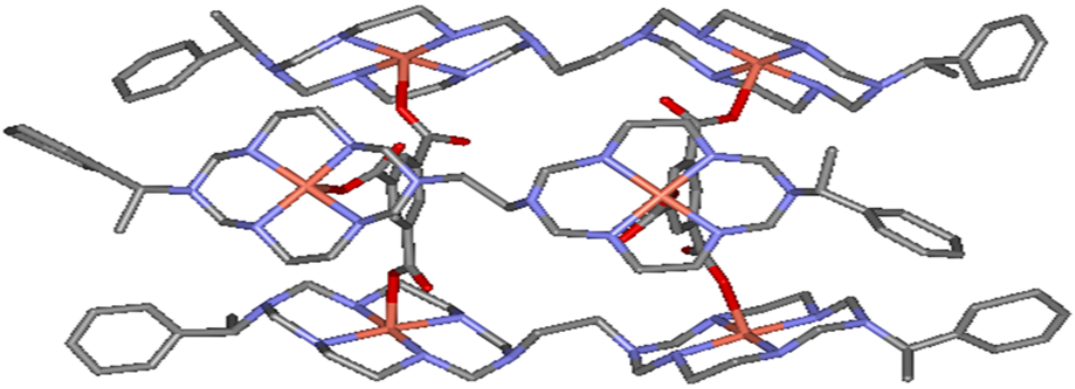
Assembly of molecular capsules from chiral dinuclear macrocyclic copper(II) complex prepared via one-pot template condensation

신종원, 로투산카라라오, *류재정, *민길식

*경북대 화학과 *경북대 사범대학 화학교육과*

Novel dinuclear macrocyclic copper(II) complexes, $[Cu_2(C_{34}H_{62}N_{12}{}^{R,R})](ClO_4)_4$ (1) and $[Cu_2(C_{34}H_{62}N_{12}{}^{S,S})](ClO_4)_4$ (2) having chiral pendant groups have been synthesized by one-pot template condensation. From the self-assembly of H_3BTC and H_3CTC with 1 and 2, new type of chiral multinuclear complexes, $[Cu_2(L^{R,R})]_3[BTC]_2{\bullet}6ClO_4$ (3) and $[Cu_2(L^{R,R})]_3[CTC]_2{\bullet}6ClO_4$ (4), have been constructed, respectively. 1 and 2 were characterized by FT-IR and FAB mass. The structures of 3 and 4 were determined by single-crystal X-ray analysis. All copper(II) ions in 3 and 4 show square pyramidal geometries. In case of 3, it shows a cage structure. In this poster, the detailed preparation, crystal structure, and properties of 1-4 will be described.



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Gold-iron oxide hybrid nanoparticle as a CT/MRI dual contrast agent for in vivo hepatoma imaging

김동규, 유미경, *정용연, 전상용

*광주과학기술원 생명과학과 *전남대 영상의학과*

We report hybrid nanoparticle composed of iron oxide nanoparticle confused with gold nanoparticle as a potential CT/MRI dual contrast agent. The hybrid nanoparticle was synthesized via thermal decomposition of mixture of Fe-oleate and Au-oleylamine complexes and particles were coated with amphiphilic poly(DMA-r-mPEGMA-r-MA) by nanoemulsion method to impart water-dispersity and antibiofouling properties. In vitro phantom study, the hybrid nanoparticles had high CT intensity due to the gold nanoparticle part and good MR signal due to iron oxide nanoparticle part. Intravenous injection of the hybrid nanoparticles into hepatoma-bearing mice resulted in high contrast between hepatoma and normal liver tissue on both CT and MR images. These results suggest that the hybrid nanoparticle can be used as a CT/MRI dual contrast agent for in vivo hepatoma imaging.

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Anion-dependent chiral copper(II) complexes: Study on the structure and chirality

박아현, *신종원, *로투산카라라오, **민길식

*경남과학고 *경북대 화학과 **경북대 사범대학 화학교육과*

In an effort to explore the role of the counter anions in the preparation of mononuclear copper(II) complexes which can have three bidentate ligands potentially, new chiral copper(II) complexes of the types $[Cu^{II}(R\text{-ppme})_3](ClO_4)_2$ (1) and $[Cu^{II}(R\text{-ppme})_2(SO_4)]\bullet 4CH_3OH$ (2) (*R*-ppme = (*R*)-(+)-1-phenyl-*N*-(pyridine-2-ylmethylene)ethanamine, $C_{14}H_{14}N_2$) have been synthesized by the reactions of $Cu(ClO_4)_2\bullet 6H_2O$ and $CuSO_4\bullet 5H_2O$ with *R*-ppme in methanol under aerobic conditions. The complexes were isolated and characterized by IR, UV/Vis, EA, EPR, CD, and X-ray crystallography. Interesting things are; i) 1 was obtained as a distorted tris(bidentate)copper(II) complex easily, ii) complexes 1 and 2 show different chiralities each other, even though the bidentate ligand used has the same chirality. Herein, the detailed preparation, crystal structure, physical properties of 1 and 2 will be described.

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Conformational switching operating on platinum(II) coordination plane triggered selectively by oxalate anion

주리라

이화여대 화학나노과학과

N-Alkyl-substituted-ethylenediamine complexes of platinum(II) are well known to adopt syn and anti conformers which are inter-converted fast in aqueous solution. It is attractive to develop a conformational switching system by exploiting this behavior. Thus, we designed molecule with two uryl groups that are well known to bind carboxylates. We expected that syn and anti conformer of would be interconverted and suitable dicarboxylate anion would urge the conformation to syn form.

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Synthesis and Structure determination of titania-silica mixed oxides

박상수, *방민혁, 안병태, 황헌

*성균관대 생명공학부 *성균관대 생명공학과*

Titania-silica mixed oxide materials have received much attention over recent years because of their physical properties and lend them to a number of technological uses. These materials have been used as optical waveguides, chemical sensor, catalysts, catalyst support, and thin coatings with tailored refractive indices. The properties of titania-silica mixed oxides are strongly dependent on many condition parameters, including the composition, crystallographic structure, particle size and so on. Among those condition parameters, crystallographic structure still have not cleared because Ti-Si mixed oxide single crystals have not been easily synthesized.In this research, titanium tetraisopropoxide and tetraethoxysilane were used as the starting compound for synthesis Ti-Si mixed oxides. Each of precursors has been reacted in acidic mixed solvent ethanol and isopropyl alcohol. Ti-Si mixed oxide single crystal have been prepared and those structure have been determined by single crystal xrd. The result of crystal determination is that empirical formula is $H_{10}O_9SiTi$, crystal system is triclinic, space group is P-1, unit cell dimension s are a = 5.9521(2) Å, b = 6.1092(2) Å, c = 10.7053(4) Å, α= 77.350(2)°, β= 82.303(2)°, γ= 72.707(2)°, and volume is 361.66(2) $Å^3$.

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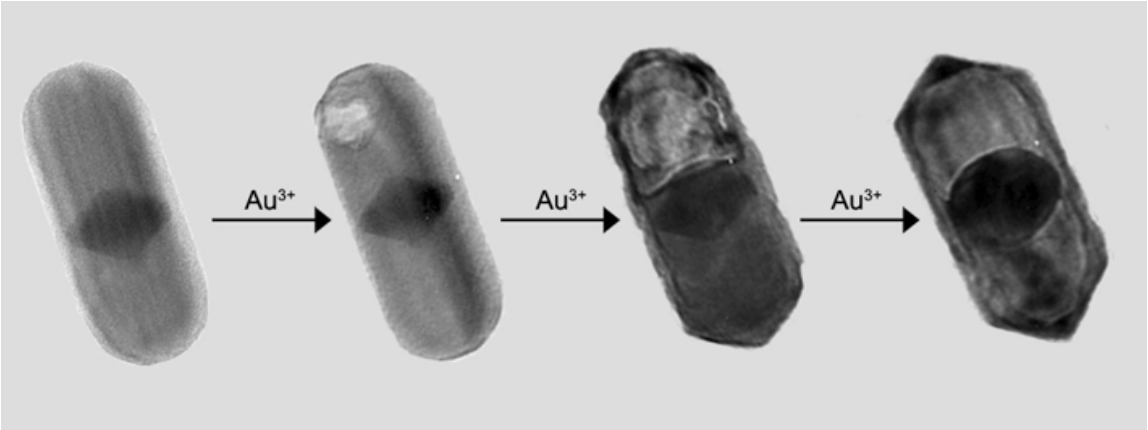
Asymmetric Hollow Nanorod Formation through a Partial Galvanic Replacement Reaction

서대하, 송현준

KAIST 화학과

Hollow nanostructures or nanocages have been used as carriers for site-specific drug delivery. In particular, metal nanocages are of critical interest due to their surface plasmon extinctions in the NIR ranges, which efficiently penetrate into biological media. The metal nanocages were commonly synthesized by metal layer deposition and the subsequent removal of templates. Xia et. al. developed nanoscale Galvanic replacement reactions, where Ag nanostructures were displaced by other noble metals to form metal hollows. However, most of the hollow structures were restricted to highly symmetrical structures, including hollow spheres, vacant regular polyhedrons, and tubes. In the present work, asymmetric hollow formation is demonstrated in a heterometal nanorod system by a partial Galvanic replacement reaction for the first time. Careful control of the reaction kinetics could yield a single hollow on one side as well as a double hollow on both sides of silver domains in the Ag-Au-Ag nanorod structure.



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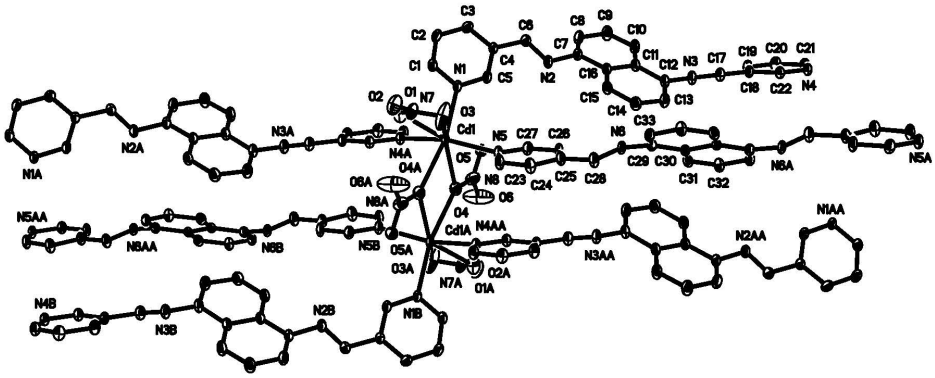
Ligand 환경에 따른 배위능력 비교와 구조 이성질체 관계의 ligand 에 의한 mixed ligand coordination polymer: $[Cd_2(L^1)_2(L^2)(NO_3)_4]_\infty$, $\{L^1 = (3\text{-py})\text{–CH=N–}C_{10}H_6\text{–N=CH–}(3\text{-py});\ L^2 = (4\text{-py})\text{–CH=N–}C_{10}H_6\text{–N=CH–}(4\text{-py})\}$

정영민, 이순원

성균관대 화학과

우리는 Polymer 1 $[Cd_2(L^1)_2(L^2)(NO_3)_4]$, Polymer 2 $[Cd(L^1)_2(NO_3)_2]$, Polymer 3 $[Cd(L^2)_{1.5}(NO_3)_2]$를 합성하고, ligand 사이의 배위능력을 비교하였다. 이 연구에서 우리는 4 개의 리간드의 배위능력을 조사하였다. 사용된 리간드는 L^1 (L^1 = (3-py)–CH=N–$C_{10}H_6$–N=CH–(3-py)), L^2 (L^2 = (4-py)–CH=N–$C_{10}H_6$–N=CH–(4-py)), L^3 (L^3 = (3-py)–CH_2–NH–$C_{10}H_6$–NH–CH_2–(3-py)), L^4 (L^4 = (4-py)–CH_2–NH–$C_{10}H_6$–NH–CH_2–(4-py)) 이다. L^1 과 L^2 사이의 비교실험에서는 서로 우열을 나타내지 않고 Polymer 1 안에 함께 배위했다. L^1 과 L^3, L^2 와 L^4 사이의 비교 실험에서는 imine group 이 존재하는 L^1 과 L^2 가 우세를 보였다. Polymer 2 와 Polymer 3 는 기존에 알려진 화합물이 합성되었고, polymer 1 은 cadmium dimer 를 함유한 2 차원 평면 구조를 형성하였다. 이러한 결과에 의해 우리는 두 가지 결론을 내렸다: (1) 말단 pyridine 의 질소 원자 위치는 리간드의 배위 능력에 큰 영향을 주지 못한다. (2) 리간드 내의 imine 그룹이 환원될 경우 리간드 전체의 배위 능력이 크게 떨어진다.Keywords: Mixed ligand coordination polymer ; Constitutional isomer; Reduced ligands; Coordination ability



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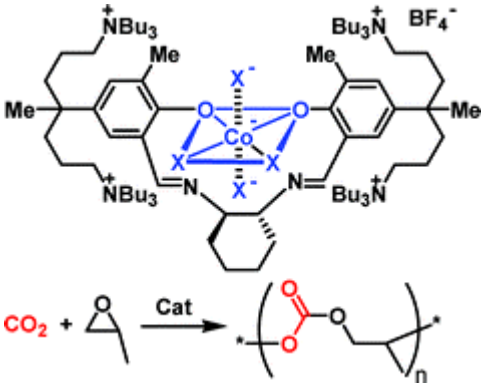
Anion variation on a cobalt(III) complex of salen-type ligand tethered by four quaternary ammonium salts for CO_2/epoxide copolymerization

도승현

아주대 응용화학과

Anion exchange of BF_4^- occurs by stirring a cobalt(III) complex of salen-type ligand tethered by four quaternary ammonium BF_4^- salts over a slurry of NaX in CH_2Cl_2, affording a complex containing four X's per cobalt (X = 2,4,5-trichlorophenolate, 6; X = 4-nitrophenolate, 10; X = 2,4-dichlorophenolate, 12). The ^1H and ^{13}C NMR spectra are in agreement with an unusual imine uncoordinated structure. The two salen-phenoxys and the two X's persistently coordinate with cobalt(III) to form a square planar cobaltate complex while the other two X's scramble through coordination and decoordination to the axial sites of the square plane. Another form of the complex (X = 2,4,5-trichlorophenolate, 14; X = 4-nitrophenolate, 15; X = 2,4-dichlorophenolate, 16) is also prepared, in which the scrambling two X's in 6, 10, or 12 are replaced with the corresponding $[XHX]^-$ homoconjugate. These complexes, which adopt an unusual imine uncoordinated structure, are excellent catalysts for CO_2/propylene oxide copolymerization (turnover frequency (TOF), 8300-16000 h^{-1}). In all cases, the complex containing the homoconjugate $[XHX]^-$ shows higher activity than the corresponding phenol-free complex. Among the prepared complexes, 4-nitrophenol-4-nitrophenolate homoconjugate complex 15 showed the best performance (TOF, 16000 h^{-1}; selectivity, 98%; Mn, 273000), allowing for replacement of the explosive 2,4-dinitrophenolate complex.



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A stable radical cation of dyes using the fused-sulfur

김철우, 김철우, 김철우, 소슬기, 소슬기, 소슬기, *유태정, *유태정, *유태정, 강상욱, 강상욱, 강상욱, 고재중

*고려대 소재화학과 *고려대 신소재화학과*

Some p-substituted triphenylamine radical cations are stable species in a propeller-like structure in solid state. However, the unsubsitituted triphenylamine shows an irreversible oxidation peak in its cyclic voltammogram, indicating that the radical cation has much poorer stability. In order to obtain insight into their electron-donating ability and stability, we have investigated the lesser bridged triphenyl amines, 2,2':6',2''-dithiatriphenylamine. We were to get the JK-126, JK-150 contained 2,2':6',2''-dithiatriphenylamine.

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Ion-coordinating ruthenium sensitizers for dye sensitized solar cells containing aza-crown ether group

조나라, 정반석, 강상욱, 고재중

고려대 소재화학과

Ion-coordinating ruthenium sensitizers (JK-122 and JK-122) containing aza-crownether group were synthesized and characterized. Using these sensitizers, we obtain a photovoltaic efficiency of 7.17 % and 6.49 % under AM 1.5, respectively. The influence of lithium cation present in the electrolyte on the device photovoltaic parameters was studied, and the FTIR spectral and photovoltage transient study showed that lithium cation coordinate to the aza-crown ether groups on the JK-121 and JK-122 sensitizer molecules.

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Development of New Bridging Group and Organic Sensitizer for Solar Cells

임기민, 백상현, 최현봉, 강상욱, 고재중

고려대 소재화학과

Dye-sensitized solar cells (DSSCs) are currently attracting considerable academic and industrial interest as low-cost, high-efficiency alternatives to the conventional silicon p-n junction photovoltaic devices. We designed and synthesized new organic dyes, which have a fluorene derivative as donating group and cyanoacrylic acid as withdrawing group and dithienothiocyclopentane as bridging group. We expected that absorption spectra and efficiency are increase. Consequently we can synthesize and develop an efficacious bridging group through in this study.

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Donor Effect of Organic Sensitizers with planarity

백상현, 최혜주, 최현봉, 최홍식, 강상욱, 고재중

고려대 소재화학과

Dye-sensitized solar cells(DSSCs) based on nanocrystalline semiconductor have been intensively studied because of their potential low-cost, easy processing and high performance. Recently, we report two organic sensitizers, coded JK-180 and JK-186. Successful molecular engineering were achieved by incorporating alkyl or alkoxy units into the organic framework with a planar hexylthienothiophene–vinylene–hexylthienothiophene as linker. In THF solution, the absorption maxima peak shows at 492nm, 494nm, respectively. Compare with JK-112(480nm), these dyes are red-shifted. Consequently cause of donating ability. We expect to get high power conversion efficiency.

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High efficiency dye-sensitized solar cells with an organic chromophore featuring a π-conjugated spacer

도광석, 정반석, 최홍식, *고혜민, 강상욱, 고재중

*고려대 소재화학과 *서울대 화학부*

Dye-sensitized solar cells (DSSCs) are currently attracting considerable academic and industrial interest as low-cost, high-efficiency alternatives to the conventional silicon p-n junction photovoltaic devices. It have been used not only transition metal complex but also organic dye as photosensitizers for dye-sensitized solar cells. JK-192 and JK-193 containing long alkyl chain attached fused-amine for donor group are designed and synthesized. Under standard global AM 1.5 solar condition, We found that the η of JK-192 was higher than η of JK-193 due to the higher Voc and Jsc. The improved Voc and Jsc value is attributed to the suppression of dark current owing to the blocking effect of a long alkyl chain at donor and spacer.

일시: 2010년 4월 29~30일(목~금) 2일간
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발표코드: **Ⅲ33P72포**
발표분야: 무기화학
발표종류: 포스터, 발표일시: 금 10:30~12:30

Organic Sensitiser Containing Perylene Imides for Efficient Panchromatic DSSCs

김경준, 최현봉, 최홍식, 강상욱, 고재중

고려대 소재화학과

Molecular photovoltaic devices with extended absorption in the near-IR region of the spectrum are currently a hot topic in the area of solar cells. We have focussed on perylene imides as good sensitizers for DSSCs due to their outstanding chemical, thermal and photophysical stabilities. Moreover perylene imides exhibit very high extinction coefficients around 700nm for efficient photon harvesting but the light-to energy conversion efficiency values remain low compared with other organic dyes. For that reason, we introduced organic dye that consist of the bis-dimethylfluoreneaniline moiety acting as electron donor and the two functions being connected by conducting thiophene units.

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발표종류: 포스터, 발표일시: 금 10:30~12:30

Mixed-Ligand MOFs Exhibiting Very Large Surface Areas

고낙은, 최상범, 조은희, 강은영, 김자헌

숭실대 화학과

The use of elongated organic linkers that are assembled with well-defined inorganic clusters, such as Zn_4O clusters, is an easy approach for increasing the surface areas of MOFs. However, this method is usually accompanied by interpenetration or weaker frameworks so that the surface areas of the resulting MOFs are reduced. In this poster presentation, this problem was overcome using a judicious combination of two different linkers, ditopic and tritopic carboxylates, in order to obtain non-interpenetrating, highly-porous MOFs. The crystal structures and porosity data for the four Zn-MOFs was presented and discussed in terms of the framework design. One of these MOFs had BET and Langmuir surface areas of 6240 and 10400 m^2/g, respectively.

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발표분야: 무기화학
발표종류: 포스터, 발표일시: 금 10:30~12:30

High Molar Extinction Coefficient Organic Sensitizers for Efficient Dye-Sensitized Solar Cells

최현봉, 김철우, 백상현, 조나라, 임기민, 도광석, 최혜주, 소슬기, 김경준, 최홍식, 정반석, *유태정, 강상욱, 고재중

*고려대 소재화학과 *고려대 신소재화학과*

We have designed and synthesized highly efficient organic sensitizers with a planar thienothiophene–vinylene–thienothiophene linker. Under standard global AM 1.5 solar conditions, the JK-113-sensitized cell gave a short circuit photocurrent density (Jsc) of 17.61 mAcm2, an open-circuit voltage (Voc) of 0.71 V, and a fill factor (FF) of 72%, corresponding to an overall conversion efficiency (h) of 9.1%. The incident monochromatic photo-to-current conversion efficiency (IPCE) of JK-113 exceeds 80% over the spectral region from 400 to 640 nm, reaching its maximum of 93% at 475 nm. The band tails off toward 770 nm, contributing to the broad spectral light harvesting. Solar-cell devices based on the sensitizer JK-113 in conjunction with a volatile electrolyte and a solvent-free ionic liquid electrolyte gave high conversion efficiencies of 9.1% and 7.9%, respectively. The JK-113-based solar cell fabricated using a solvent-free ionic liquid electrolyte showed excellent stability under light soaking at 60 8C for 1000 h.

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발표종류: 포스터, 발표일시: 금 10:30~12:30

Organic Sensitizer Containing π-conjugated spacer for DSSCs

최혜주, 백상현, 강상욱, 고재중

고려대 소재화학과

Dye sensitized solar cells(DSSCs) are currently attracting wide-spread interest as low-cost alternatives to conventional solid-state photovoltaic devices. Controlling the light harvesting in DSSCs is very important due to the scientific and industrial interest to enhance the photoenergy conversion efficiency. We introduce thieno[3,2-b]thiophene group, we expect to increase planarity and enhanced π-electron delocalization. For increasing Voc, we introduced to hexyl group. JK-182 gave increase of Voc value compared with JK-181. However, the JK-182 gave decrease of Jsc and conversion efficiency compared with the JK-181.

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발표종류: 포스터, 발표일시: 금 10:30~12:30

Synthesis, crystal structure, and magnetic properties of (μ-oxo)diiron(III) complexes with mono-/bidentate and bi-/tridentate ligands

로투산카라라오, 신종원, *민길식

*경북대 화학과 *경북대 사범대학 화학교육과*

The thermodynamically stable (μ-oxo)diiron(III) complexes with organic ligands are important because of their interesting electronic structures and the magnetic interactions between the two iron(III) centers and the role they play in dioxygen binding. Due to this interest we have synthesized two dinuclear iron(III) complexes with an oxo-bridged, $\{[Fe(S\text{-}pbpe)(NCS)]_2(\mu\text{-}O)\}$ (1) and $\{[Fe(tpa)(3,4\text{-}dhbn)]_2(\mu\text{-}O)\}$ (2) from the reaction of $[Fe^{II}(H_2O)_6]\bullet(BF_4)_2$, (S)-1-phenyl-N,N-bis(pyridin-2-ylmethyl)ethanamine (S-pbpe), NaSCN in methanol and $[Fe^{III}(H_2O)_9]\bullet(NO_3)_3$, tris(2-pyridylmethyl)-amine (tpa), 3,4-dihydroxybenzonitrile (3,4-dhbn) and triethylamine in methanol, respectively. The crystal structures of 1 and 2 have been determined by single-crystal X-ray analysis. Herein, the detailed preparation, crystal structure, magnetic properties of 1 and 2 will be presented.

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발표종류: 포스터, 발표일시: 금 10:30~12:30

Synthesis and optical properties of organometallic complexes based tetrazine ligand

김윤희, 나영준, *최문근

*연세대 화학과 *연세대 이과대학 화학과*

The search for new functional organic materials is still very active. Among desirable features to achieve, fluorescence as well as the ability to exchange electrons is among the preferred ones, especially when they can be coupled together. We became interested into original molecules, molecular materials and polymers based on tetrazine rings. The tetrazine ring is the most electron deficient aromatic ring in the CHON chemistry. Its electron deficient character also allows the tetrazine ring to be reversibly reduced by removing one or even two electrons, and thus opens towards the fabrication of electron transferring polymers or switchable fluorescent materials and devices. Some aspects on the fluorescence of original molecules, molecular materials and polymers based on tetrazines rings, are particularly interesting, and could be enhanced by coupling with other systems such as organometallic systems. Organometallic systems combine also usually a redox property to light absorption, but the introduction of a metal into an organic molecule can also modify the electron density, and therefore change the property of the molecule.The aim of this study is synthesis of tetrazine ligands and preparation of their organometallic complexes for studies of their photophysical properties.

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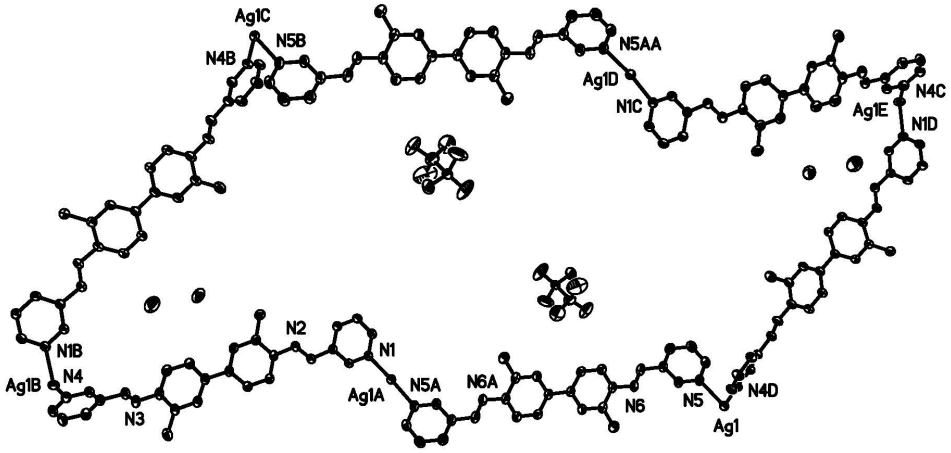
발표종류: 포스터, 발표일시: 금 10:30~12:30

Homoleptic silver–bis(pyridine) coordination polymers: $[Ag(L^1)_2]\bullet(PF_6)$, $[Ag(L^1)_2]\bullet(SbF_6)$, $[Ag(L^1)_2]\bullet(BF_4)$, $[Ag(L^2)]\bullet(PF_6)$, and $[Ag(L^3)_{1.5}]\bullet(CF_3SO_3)\bullet(H_2O)_2$ {L1 = (4-py)–CH=N–$C_{10}H_6$–N=CH–(4-py); L2 = (2-py)–CH=N–$C_{10}H_6$–N=CH–(2-py); L3 =(3-py)–CH=N–$C_{14}H_{12}$–N=CH–(3-py)}

장영옥, 이순원

성균관대 화학과

Five homoleptic silver–bis(pyridine) coordination polymers, $[Ag(L^1)_2]\bullet(PF_6)$ (1), $[Ag(L^1)_2]\bullet(SbF_6)$ (2), $[Ag(L^1)_2]\bullet(BF_4)$ (3), $[Ag(L^2)]\bullet(PF_6)$ (4), and $[Ag(L^3)_{1.5}]\bullet(CF_3SO_3)\bullet(H_2O)_2$ (5), were prepared from AgX (X = PF_6, SbF_6, BF_4, CF_3SO_3) and rigid bis(pyridine)-type linking ligands {L1 = (4-py)–CH=N–$C_{10}H_6$–N=CH–(4-py); L2 = (2-py)–CH=N–$C_{10}H_6$–N=CH–(2-py); L3 =(3-py)–CH=N–$C_{14}H_{12}$–N=CH–(3-py)}. Polymers 1–3 are isostructural and have the same non-interpenetrated, 3-D diamondoid framework, whose cavities are almost completely filled with the counterions. Polymer 4 is a 1-D chain polymer. Polymer 5 is a 2-D -arsenic-type polymer with a repeat unit of a 114-membered ring.



THE KOREAN CHEMICAL SOCIETY

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장소: 송도컨벤시아
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발표분야: 무기화학
발표종류: 포스터, 발표일시: 금 10:30~12:30

Blue Phosphorescence Ir(III) Complex; Structure, Optical Properties and DFT calculation of mer-Ir(dfbpy)3 (dfbpy=2′,6′-difluoro-2,3′bipyridine-N^C′)

강영진, *이은지, *김진호, *정나래

*강원대 과학교육과 *강원대 화학과*

Luminescent complexes containing third-row transition metals have attracted much attention owing to varied applications, such as photonics and electronics. Especially, cyclometallated Iridium(III) complexes regarded as excellent phosphorescent materials have been widely studied because of their ability to achieve maximum internal quantum efficiency, nearly 100%, as well as high external quantum efficiency in OLEDs. As reported previously, to be a promising phosphorescent metal complex in OLEDs, the complex should have high thermal stability and phosphorescent efficiency. Cyclometallated (C^N)3Ir(III) complexes with facial geometry are satisfactory to these considerations, and hence their derivatives were widely investigated. In particlar, luminescent Ir(ppy)3 (ppy = 2-phenylpyridine) derivatives have been described where adjustment of the band gap between the HOMO and LUMO energy levels could be achieved by the simple modification of the ppy rings. Our interest in the development of highly efficient phosphors for the application in OLEDs has prompted us to synthesize and investigate the photophysical and electroluminescent characteristics of Ir(ppy)3 derivatives. Herein we describe the results of our investigation on the preparation, structural characterization, photophysical properties and DFT calculation of a new homoleptic fac-tris(dfbpy)3Ir(III) (dfbpy = 2′,6′-difluoro-2,3′-bipyridine-NΛC2) complexe.

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발표분야: 무기화학
발표종류: 포스터, 발표일시: 금 10:30~12:30

Fabrication of Highly Luminescent InP/Cd and InP/CdS Quantum Dots

박재현

아주대 분자과학기술학과

Highly luminescent InP/Cd and InP/CdS core-shell QDs were fabricated by sequential addition of cadmium acetylacetonate and dodecanethiol to InP core solutions, which showed a red-shift in absorption and emission. ICP measurement revealed the existence of cadmium and TEM images showed the increased size of InP/CdS QDs. PXRD data identified zinc blend structures of InP and InP/CdS QDs, which indexed to the (111), (220) and (311) planes. The slight shift of peaks between InP and InP/CdS QDs can demonstrate the existence of CdS shell structures.

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발표종류: 포스터, 발표일시: 금 10:30~12:30

Dehydration of D-xylose to furfural with γ-Al2O3 modified with propylsulfonic acid group

김은규

아주대 분자과학기술학과

All types of γ-Al_2O_3 such as acidic, neutral and basic form were chemically modified with (3-mercaptopropyl) trimethoxysilane (3-MPTMS) and oxidized by 30wt% H_2O_2 solution. As a result, propylsulfonic acid modified γ-Al_2O_3(γ-As) were obtained. All types of γ-Al_2O_3 are more easily modified with treating 1M HCl. Their catalytic performance was tested by dehydration reaction of D-xylose to furfural. All catalytic reaction indicated fairly increased conversion of D-xylose. As increasing propylsulfonic acid group of catalysts, selectivity to furfural is also increased.

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발표종류: 포스터, 발표일시: 금 10:30~12:30

Synthetic, cyclic voltammetric, structural, EPR and UV-vis spectroscopic studies of thienyl-containing meso-A_2B-cor(CrV=O) systems.

Tsay Olga, *D.G.Churchill

*KAIST 화학과 *KAIST 화학과*

Corrolate (cor) systems, especially A_3-tris(pentafluorophenyl)corrole- or (tpf)cor-based ones are, by now, relatively well-known ligands, with many reports relating to metal-mediated catalysis. This foray has reaped various related ligands and metal complex derivatives alike, as well as subsequent metal-based axial ligands (e.g., M=O, M=N-R), which, in corrole chemistry, posses properties and reactivites that, unlike in the porphyrin literature, are still being studied and established. The terminal oxo- and closely-related derivatives are of great research interest as potential motifs in “compound I” modeling with small molecules. We endeavor to expand the potential of these contracted porphyrins as possible useful solution-based polypyrrolic probes through considerations of the interrelationships of the free base, the metal complex, and the terminal oxo derivative.We have synthesized new A_2B-corroles and report novel Cr=O species. These derivatives represent the first examples of meso-A_2(thienyl) and Cr-A_2B-corrole types. The formal replacement of one $-C_6F_5$ group with one thienyl substitution was expected to change the extreme electron-withdrawing nature known for the tris-C_6F_5-A_3-type tpf(cor) species. This thienyl substitution also allows for an adjacent ligand-based oxidation site at the sulfur. Chromium was selected for incorporation because of its redox utility. The structures of compounds have been characterized by a number of physical methods including UV-vis, 2-D (1H, 13C) NMR, EPR spectroscopy, mass-spectrometry, elemental analysis and cyclic voltammetry. Also, two single-crystal X-ray crystallographic studies were performed, in addition to obtaining a measure of the catalytic reactivity of the new corroles.

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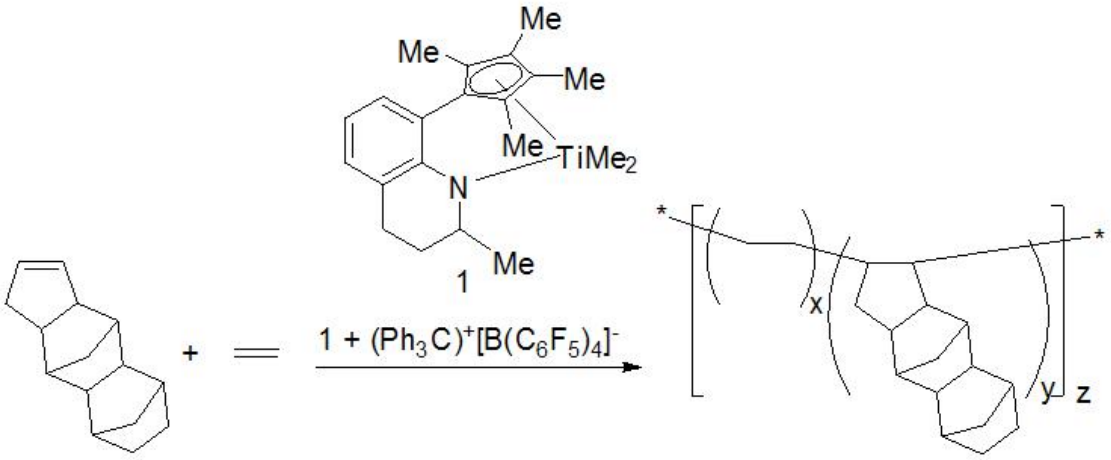
발표종류: 포스터, 발표일시: 금 10:30~12:30

Copolymerization of 5,6-Dihydrodicyclopentadiene and Ethylene

박형철

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-(h5-C_5Me_4)-2-Me(C_9H_8N)-kN]$TiMe_2$ ($C_9H_{10}NH$ = 1,2,3,4-tetrahydroquinoline) activated with (Ph_3C)+[$B(C_6F_5)_4$]-. The copolymer was unambiguously characterized through the analysis of one- and two-dimensional NMR spectra. The monomer reactivity ratios, rethylene and rHTCPC, determined through the Fineman-Ross plot, were 2.8 and 0.025, indicating successive insertion of two HTCPD is negligibly allowed. A nearly alternating copolymer with HTCPD content of 45 mol% was obtained with a satisfactory activity (4.7 ×10^6 g/molTi·h), of which Tg is 177℃, significantly higher than that of norbornene/ethylene copolymer at the same cycloolefin content. Tensile stress-strain curves indicated that the brittleness observed for a high Tg norbornene/ethylene copolymer was relieved to show some ductile property for HTCPD/ethylene copolymer of the same level of high Tg.



일시: 2010년 4월 29~30일(목~금) 2일간
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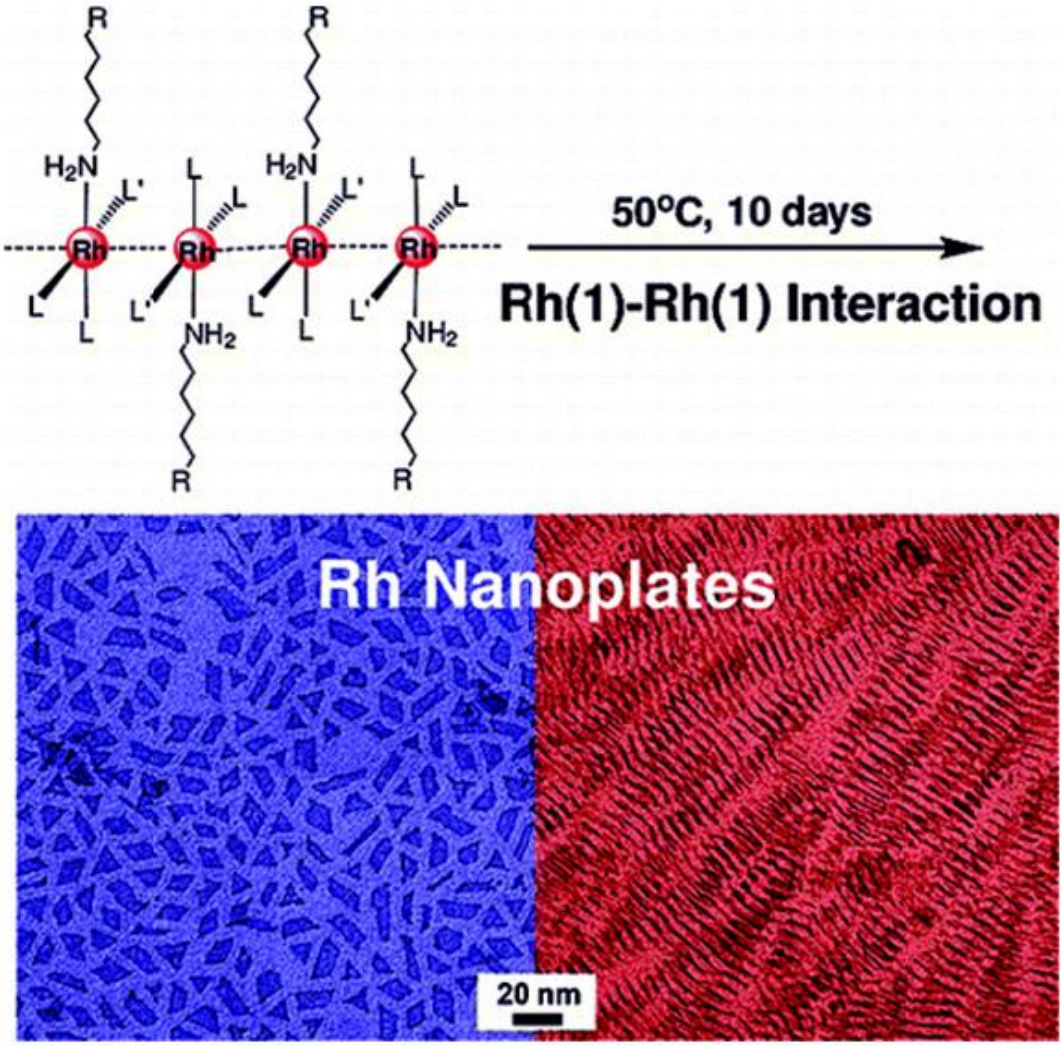
Shape-controlled Synthesis of Ultrathin Rhodium Nanoplates via Molecular Orbital Symmetry Interaction between Rhodium Precursors.

장권호, 손성욱

성균관대 화학과

Shape-controlled synthesis of nanomaterials has become an important issue to synthetic material scientists because new physical and chemical properties can be obtained through the evolution of unprecedented shapes. The Xia and Yang groups demonstrated the growth of gold nanowires in amine solution at low temperature. The cubic phase of the resultant nanowires indicates that the low-temperature growth has the potential to produce unprecedented nanomaterials. Interestingly, the relatively weak Au-Au aurophilic interaction in solution played a key role in the assembly of precursors and the resultant shape evolution. Similar to the aurophilic interaction, a weak metal-metal interaction between the group 9 metals with an oxidation state of +1 was observed by Gray and coworkers, which has been attributed to a molecular orbital symmetry interaction of the filled σ-metal-metal bonding and σ*-antibonding orbitals with the empty pz σ and σ* orbitals. This interaction stabilized the filled orbitals and destabilized the empty orbitals. Despite its relative weakness, the resultant interaction is strong enough to induce the assembly of complexes, even in solution. Very recently, our research group disclosed the Rh(I)-Rh(I) interaction of square planar Rh(CO)2Cl-(amine) complexes to form molecular wires. In the present study, we report the preparation of unprecedented ultrathin (1.3 nm thickness) rhodium nanoplates at 50 oC via metal-metal interaction between Rh(I) precursors.



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발표분야: 무기화학
발표종류: 포스터, 발표일시: 금 10:30~12:30

Highly Uniform Superparamagnetic Mesoporous Silica Spheres Embedded with FeCo-Graphite Nanocrystals

LIYAN, *김연진, *서원석

*서강대 바이오융합 *서강대 화학과*

We have synthesized highly uniform superparamagnetic mesoporous silica spheres embedded with FeCo-graphite nanocrystals. Solid core-mesoporous shell silica spheres with an average diameter of ~500 nm were used as templates. FeCo-graphite nanocrystals were grown within mesoporous shells of the host silica spheres by a simple one-step CVD process. The size and number of FeCo-graphite nanocrystals were increased as the concentration of FeCo precursors in silica spheres was increased. The superparamagnetic mesoporous silica spheres were characterized by XRD, TEM, and SQUID. The superparamagnetic silica spheres exhibited stability against HCl etching over a monitoring period of a week. By exploiting the chemical stability and superparamagnetic properties, the silica spheres are expected to show novel applications including biological affinity separations, drug delivery, magnetic-resonance imaging, and catalytic supports.

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Synthesis and Characterization of Core-shell Structured FeCo/graphite/SiO2/TiO2 Nanocomposites

정주열, 최인애, 서원석

서강대 화학과

Core-shell structured FeCo/graphite/SiO2 and FeCo/graphite/SiO2/TiO2 nanocomposites with an average diameter of ~38 nm have been synthesized by combining CVD and sol-gel processes. 6 nm FeCo/single graphite shell nanocrystals, prepared by a simple CVD process, were used as seeds for the formation of ~15 nm SiO2 and 1~2 nm TiO2 shells. Tetraethyl orthosilicate (TEOS) and titanium tetrabutoxide were used as precursors for the SiO2 and TiO2 shells, respectively. The nanocomposites are expected to show novel applications including drug delivery, magnetic-resonance imaging, and catalytic supports.

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발표종류: 포스터, 발표일시: 금 10:30~12:30

Multi-way aqueous OFF-ON fluorescent salicylaldehyde, Zn2+, or amino acid detection via in situ Schiff base assembly: a "blue triangle" resource for fluorescent biological studies involving benzaldehydes

박현영, *D.G.Churchill

*KAIST 화학과 *KAIST 화학과*

Zn2+ is ubiquitous in biology and is a greatly pursued analyte (especially in neuroscience). During zinc "bursts" common during neurotransmission, various unnatural binding could restrain Zn2+ from playing its natural neuroprotective role. Thus, an understanding of which species form under what conditions at what wavelengths (abs/em) is essential. Previously, we reported that the complex composed of Zn2+, D/L-lysine (Lys) and salicylaldehyde (Sal) exhibited strong blue fluorescence (λem,max = 450 nm). Currently, we probe in situ fluorescent Zn2+-Schiff base complex formation using D/L-lysine (Lys) and 2,3- diaminopropionic acid (DAP) for longer durations (~ 4-24 h); these signify a three-way ambient room temperature "off-on" detection (at 50 μM conc.); three main titrations (type I: [HSal + Lys] titrated by Zn2+, type II [HSal + Zn2+] titrated by Lys, and type III ([Lys + Zn2+] titrated by HSal) separately demonstrated detection for Zn2+ (79-fold increase), and D/L-lysine (96-fold increase) / 2,3-diaminopropionic (26-fold increase) and Sal (82-fold increase) at, e.g., 2 equiv, and 24 h, respectively. No / little fluorescence intensity arises by the absence / exchange of one component: other Mn+ ions (e.g., Mg2+, Cu2+, Hg2+), simple non-salicylaldehyde-type aldehydes, or 2°- or 3°-amines. Kinetically, lysine progresses beyond that (F.I.) for 2,3-diaminopropionic acid (no progress after 4 h). This research shows that a "triangle" of reagents is necessary for complex formation to determine the extent of Zn2+ chelate formation; a consideration of salicalydehyde detection, and opens a consideration of selective amino acid detection.

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발표분야: 무기화학
발표종류: 포스터, 발표일시: 금 10:30~12:30

Mechanochemical versus sol-gel silica loading of phenolate- and acetate-bridged dizinc complexes: toward instant and inexpensive hybrids for controlled binding and release of Zn^{2+} in pure water

전태홍, *강지나, D.G.Churchill

*KAIST 화학과 *KAIST 화학과*

Herein, we have explored expeditious and lowered expense SiO_2-loading in the context of fluorescent "off-on" and "on-off" Zn^{2+} ion detection / controlled release. A simple racemic ligand (H_2rlys) (1) prepared in situ can be mechanically SiO_2-loaded so to induce surface- sites that allow for "off-on" fluorescence (λem,max = ~450 nm) of aqueous detection Zn^{2+}; with Cu^{2+} as a competing input, "inhibit" logic gate behaviour is present. Oppositely, dimeric, chiral fluorescent zinc complexes (ϕF = ~0.20) prepared in a "one pot" method, and bearing different Zn•••Zn internuclear spacings, can be incorporated into silica by two methods. Specifically, the chiral $Zn_2(slysH)_2Cl_2$ (2) and racemic $Zn_2(rslysH)_2(\mu\text{-}OAc)_2$ species (3) [slys or rslys = 6-amino-2-{(2-hydroxybenzylidene)amino}hexanoate] were mechanochemically loaded. An adsorption constant was 1.99×10^{-4} (molecules of 2 / units SiO_2)$(min)^{-1}$ for times of 5-20 min, as determined by extensive SEM-EDS data. These confirmed highly selective "on-off" rapid aqueous fluorescent Cu^{2+} detection (versus, Li^+, Na^+, Cs^+, Mg^{2+}, Ca^{2+}, Mn^{2+}, Fe^{2+}, Co^{2+}, Ni^{2+}, Ag^+, Cd^{2+}, Hg^{2+}, Pb^{2+}) through direct Zn^{2+} displacement under bulk neat water flow (pH = 7.4) as verified by an authentic sample of $[Cu_2(slysH)_2(NO_3)_2]$-Silica (4-Silica). With use of 2•SiO_2, Na_4EDTA and Cu^{2+} "inhibit" logic gate behaviour was also found. Sol gel techniques allowed for loadings of 2 (20-890 mg) up to 1:1 (by wt). The preparation of these inorganic hybrids are extremely inexpensive and rapid to prepare from commercial starting materials and can be extended to variegated forms of SiO_2; alumina gel was also functionalized with 2. Cu^{2+} and Zn^{2+} are metals pertinent to human neurological health promotion and in neurodegenerative diseases.

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발표종류: 포스터, 발표일시: 금 10:30~12:30

A porous 3D Co-Cu bimetallic material constructed from a metalloligand: structure, magnetic and sorption properties

유대원, 이진욱, 홍창섭

고려대 화학과

A porous 3D material, $[Co(Tt)_2Cu_6(5\text{-hydroxyisophthalate})_6]\cdot xDMF\cdot xH_2O$ (1), has been synthesized by a solvothermal reaction of Cu(Ⅱ) ion, 5-hydroxyisophthalic acid, and $Co(Tt)_2$ [Tt^-=tris(1,2,4-triazolyl)borate] in mixed solvent of H_2O, MeOH, and DMF. Single crystal structure contains copper paddle-wheel secondary building unit (SBU). Each SBU is connected to nearby SBUs through metalloligands. We will present the structure, sorption and magnetic properties of (1) in the presentation.

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발표종류: 포스터, 발표일시: 금 10:30~12:30

Solvothermal Synthetic approach to $A_2Hg_3Se_4$ and $A_2Hg_2Se_3$ (A = K, Rb)

김선진, 김강우

인천대 화학과

Ternary metal selenide compounds, $A_2Hg_3Se_4$ (A = K, Rb) and $A_2Hg_2Se_3$ (A = K, Rb) have been successfully synthesized by the solvothermal method using ethylenediamine(en) as a solvent. Crystal structures of $K_2Hg_3Se_4$ and $K_2Hg_2Se_3$ compounds were determined by the single crystal X-ray diffraction method. Red rectangular thin plate crystals of $K_2Hg_3Se_4$ crystallize in the orthorhombic space group Pbcn (no. 60) with a = 10.858(2) Å, b = 6.786(1) Å, c = 14.087(2) Å, Z = 4, V = 1038.0 $Å^3$. Black rod-like crystals of $K_2Hg_2Se_3$ crystallize in the tetragonal space group P42/ncm (no. 138) with a = 15.091(1) Å, c = 7.124(1) Å, Z = 4, V = 1622.4 $Å^3$. $K_2Hg_3Se_4$ contains one-dimensional $[Hg_3Se_4]_n^{2n-}$ chains and $K_2Hg_2Se_3$ is composed of novel one-dimensional $[Hg_2Se_3]_n^{2n-}$ columns and K^+ ions located inside and outside the columns. Details of synthetic condition and physical properties for $A_2Hg_3Se_4$ and $A_2Hg_2Se_3$ will be also presented.

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발표종류: 포스터, 발표일시: 금 10:30~12:30

Unusual Slow Magnetic Relaxation and Spin Transition in One-dimensional Chain {[Mn(salcy)][W(CN)$_8$]}[Fe(bpy)$_3$]·MeCN·H$_2$O

윤정희, 조경진, 이진욱, 이진욱, 홍창섭, 홍창섭

고려대 화학과

The design and synthesis of multifunctional magnetic materials have become one of outstanding areas of research during the past years and they have opened new possibilities for high-density storage and molecular sensors. We prepared a new one-dimensional compound, {[Mn(salcy)][W(CN)$_8$]}[Fe(bpy)$_3$]·MeCN·H$_2$O (1) including a isolated [Fe(bpy)$_3$]$^{2+}$ moiety. Compound 1 shows antiferromagnetic interaction and slow magnetic relaxation at low temperatures. Surprisingly, this compound has spin transition in solution because of the presence of the Fe (II) ion. Detailed structural and magnetic studies will be given in the presentation.

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발표분야: 무기화학
발표종류: 포스터, 발표일시: 금 10:30~12:30

Construction of various dimensional Zn based metal-organic-frameworks using dicarboxylic acids and BTB ligand.

손아람, 홍창섭

고려대 화학과

By introducing the ligand, 1,4-bis(triazol-1-ylmethyl)benzene (L), and various dicarboxylic acids, 5-R-isophthalic acid, new zinc(II) compounds (R=H, 1; R=Me, 2; R=NO_2, 3) were obtained and characterized. Two-dimensional compound (1) comprises one-dimensional chains built with both the carboxylates of isophthalates and L oriented at almost right angle. Sheet complex (2) was synthesized by the reaction between the same N-ligands and 5-methylisophthalic acid. Each two-dimensional layer structure has a tetrahedral Zn center in common. Compound (3), which exhibits one-dimensional chain structure, is composed of L, 5-nitroisophthalic acid, and Zn center. This compound also has a Td Zn center. Depending on the structure of the dicarboxylic acids, the dimension of the crystals varies. More characters of these compounds will be presented in detail.

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발표종류: 포스터, 발표일시: 금 10:30~12:30

Synthesis, Crystal Structure and Magnetic Properties of a Hydrogen-Bonded Manganese(III) Porphyrin Complex

최상엽, 유인영, 이진욱, 홍창섭

고려대 화학과

$[MnTPP(CN)_2][MnTPP(CH_3OH)_2]$ (1) [TPP = *meso*-tetraphenylporphyrin] was prepared by self-assembling the molecular precursor MnTPP•Cl and CN^- source. The crystal structure contains two mononuclear molecules constructed from $Mn^{III}TPP$ subunits and the monomers are linked by hydrogen bonding between methanol and coordinated cyanide ligands. Detailed structural and magnetic studies will be given in the presentation.

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Cyanide-Bridged One-Dimensional Fe(Ⅲ)-Mn(Ⅲ) Complexes Based on a New *mer* - Positioned Fe(Ⅲ) Cyanide Precursor : Structures and Magnetic Properties

유인영, 이진욱, 윤정희, 홍창섭

고려대 화학과

Low-dimensional magnetic systems with an anisotropic nature have been one of the hot issues among molecule-based magnetic material. The capped molecular precursors $[Fe(L)(CN)_x]^{y-}$ (L = blocking ligands, x = 2-5), where Fe(III) can act as an anisotropic center, have been utilized in the construction of magnetically interesting systems with n-dimensional structures (n = 0 and 1). A new molecular precursor, *mer* - $[Fe(4meo\text{-}iqcq)(CN)_3]^-$ (1), and two 1D chains, $[Fe(4meo\text{-}iqcq)(CN)_3][Mn(salen)]\bullet MeCN$ (2) and $[Fe(4meo\text{-}iqcq)(CN)_3][Mn(F\text{-}salen)]\bullet H_2O$ (3), were prepared and characterixed in terms of structure and magnetism. Each Fe center of the complexes adopts a distorted octahedral environment consisting of three N atoms from a planar 4meo-iqcq and three terminal CN groups. The axial elongation around Mn(III) accounts for the existence of the well-known Jahn-Teller effect on an octahedral high-spin Mn(Ⅲ) ion. However these structures are quite different each other : zigzag type chain via the cyanide-bridged consists of 2 whereas linear one consists of 3. Detailed structural and magnetic studies will be given in the presentation.

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발표종류: 포스터, 발표일시: 금 10:30~12:30

Syntheses, crystal structures, and magnetic properties of cyanide-bridged bimetallic [W(CN)$_6$(bpy)][MnL] compounds with various Schiff bases.

이진욱, 유인영, 윤정희, 홍창섭

고려대 화학과

The title compounds were prepared by self-assembly between [W(CN)$_6$(bpy)] and MnL (L_1 = 4meo-salcy, L_2 = 4meo-salen, L_3 = 4meo-salmen) in a stoichiometric ratio. The central geometry and the positions of bridging cyanides would affect magnetic coupling. The W of these compounds adopts a distorted square antiprism calculated from shape measure analysis. Therefore, their magnetic couplings are expected to be different from other [W(CN)$_6$(bpy)][MnL] (L_4 = 4meo-hadp, L_5 = 4meo-haed), which can be described as a distorted dodecahedron. Structural and magnetic characterizations for the compounds will be described in the presentation.

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발표종류: 포스터, 발표일시: 금 10:30~12:30

A 2D layered metal-organic framework from trifunctionally flexible aryl ether ligand

방원주, 홍창섭

고려대 화학과

In recent years, the design and controlled assembly of coordination frameworks based on metal centers and multifunctional bridging ligands are of great interest owing to their versatile architectures and topologies as well as potential application in a variety of areas, including catalysis, gas storage, separations, fluorescent sensing. We have synthesized a 2D layered metal-organic framework from zinc nitrate and trifunctional ligand, 1,3,5-Tri(4-carboxyphenoxy)benzene. In this framework, each 2D layer is bound via hydrogen bonding which comes from zinc-coordinated H_2O molecules. There are three ZnⅡ atoms in SBUs, which are two tetrahedrally coordinated with three different carboxylate oxygens and one H_2O molecule and one octahedrally coordinated with six different carboxylate oxygens. The framework is highly stable up to 500 ℃. We will also show the gas sorption study with this material.

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발표분야: 무기화학
발표종류: 포스터, 발표일시: 금 10:30~12:30

Syntheses, crystal structures and magnetic properties of cyano-bridged bimetallic complexes containing *fac*-Fe(III) tricyanides and Mn(III) Schiff bases.

조경진, 이진욱, 홍창섭

고려대 화학과

The use of new precursor, $[(Tp^{memt4})Fe^{III}(CN)_3]^-$ produced a tetramer molecule, $[Mn^{III}_2(Br\text{-}hadp)_2Fe^{III}_2(Tp^{memt4})_2(CN)_6]$(1), and a dimer molecule, $[Mn^{III}(3\text{-}Eto\text{-}salpn)Fe^{III}(Tp^{memt4})(CN)_3]$(2). These two complexes have been characterized by means of X-ray, IR, elemental analysis, and magnetic property. The magnetic natures on the Fe(III)–C≡N–Mn(III) skeletons of complexes prepared are different, ferromagnetic for (1), and antiferromagnetic for (2). Structure and magnetic characteristics of these compounds will be discussed in a more detail.

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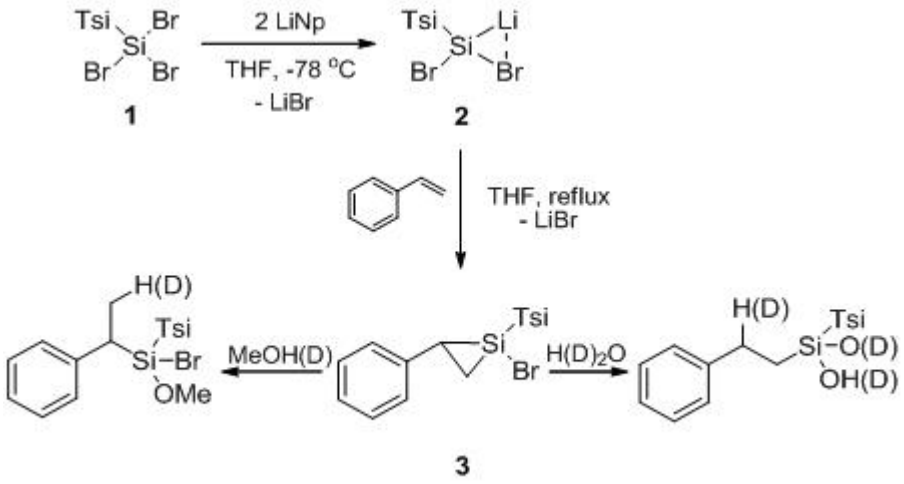
발표종류: 포스터, 발표일시: 금 10:30~12:30

Silylenoid Chemistry: Reactions of Bromosilylenoid with Olefins

복경진, *조현모, 이명의, 이명의

*연세대 화학과 *연세대 화학 및 의화학과*

Silylenoids, $TsiSiMX_2$ (Tsi = $C(SiMe_3)_3$, which contain an electropositive metal (M, alkali metals) and a leaving group (X, halogens) on silicon atom have amphiphilic properties. It has been expected that there are similarities in reactivities between silylenoids and silylenes. Reactions of silylenes with olefins reported by several groups, however, none of silylenoid has been studied. Herein, we report the reactivity of bromosilylenoid with the olefins, such as styrene and vinyltrimethylsilane, which can be one of new examples of synthetic routes for the synthesis of silacyclopropanes.The bromosilylenoid, 2 was prepared from the reaction of tribromo[tris(trimethylsilyl)methyl]silane, 1 with two equivalents of lithium naphthalenide in THF at -78 ^{o}C. To the resulting solution, an excess of styrene was added at same temperature, and then followed by the treatment of MeOH for trapping experiment to yield silacyclopropane, 3 as yellow oil. 3 was characterized by GC/MS and ^{29}Si NMR spectroscopy. Interestingly, ring cleavage occurred by MeOH and H_2O in different way. Similarly, the reaction of 2 with vinyltrimethylsilane afforded the corresponding silacyclopropane.In this presentation, we will discuss the chemistry of bromosilylenoid with olefins mentioned above in detail.



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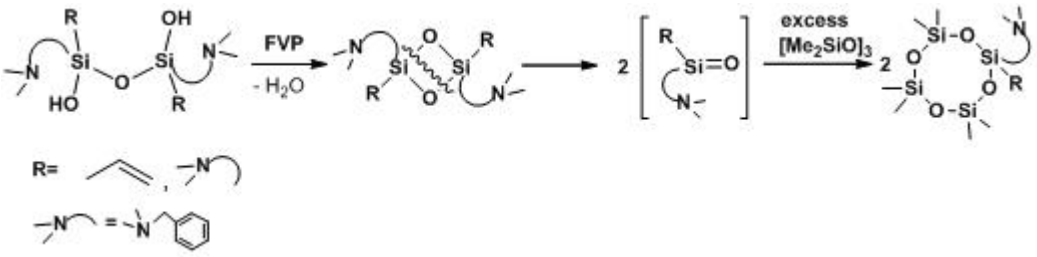
Syntheses and Reactivities of Silanones and Silanone Precursors

이수정, 임영묵, 조현모, 신동훈, 이명의

연세대 화학과

Silanone ($R_2Si{=}O$), as the silicon analogy of ketone, is known as important intermediates of silane combustion and vacuum plating in microelectronics industry. For a long time, the isolation of stable silanones had not been successful until Driess group reported the first isolable silaformamide-borane complex with considerable silicon-oxygen double-bond character. Recently, we reported the syntheses of disilanols, 1,3-dihydroxy-1,3-bis-[*o*-(*N*,*N*-dimethylaminomethyl)phenyl]-1,3-divinyldisiloxanes, bearing an intramolecular donor-atom, which could be a promising precursor for a silanone. The flow vacuum pyrolysis (FVP) of disilanols gave D_3 and D_4 products in high yields, which indicates that silanones were generated as an intermediate. The silanones were trapped by various trapping agents. In the extension of this research, we synthesized silanone precursors having intramolecular donor-atom and bulky substituents. We attempted to synthesize the stable silanone from various silanone precursors. In this presentation, these results are discussed in detail.



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장소: 송도컨벤시아
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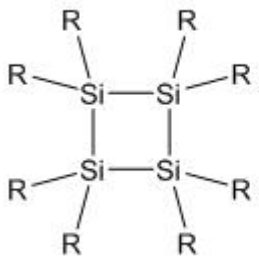
발표분야: 무기화학
발표종류: 포스터, 발표일시: 금 10:30~12:30

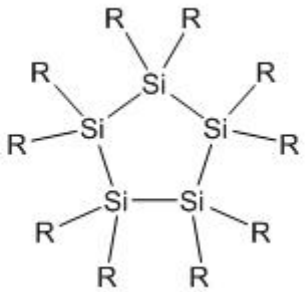
Syntheses of Cyclosilanes

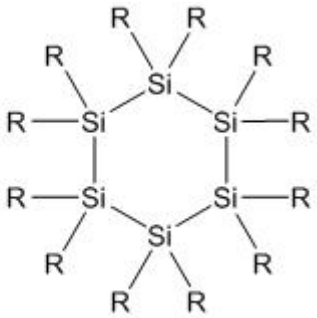
박성진, 조현모, 이명의

연세대 화학과

In cyclosilane, the delocalization of σ(Si-Si) electrons over the ring silicon atoms gives a variety of properties resembling those of aromatic hydrocarbons, such as unusually long wavelength UV absorption maxima, low ionization energies, nonlinear optical behavior, fluorescence, and photochemical activity. These compounds are particularly preferred in application fields which require high purity such as electronic materials. The cyclosilanes have been generally prepared by condensation reactions of diorganodihalosilanes. The synthetic yields of cyclic silanes depend on the choice of alkali metals and substituent groups of diorganohalosilanes. We synthesized four, five and six membered ring silanes with alkali metals under various thermal conditions. Now we are trying to apply the various cyclic silanes to the industrial field. In this presentation, the syntheses of cyclic silanes and their properties will be discussed, in detail.







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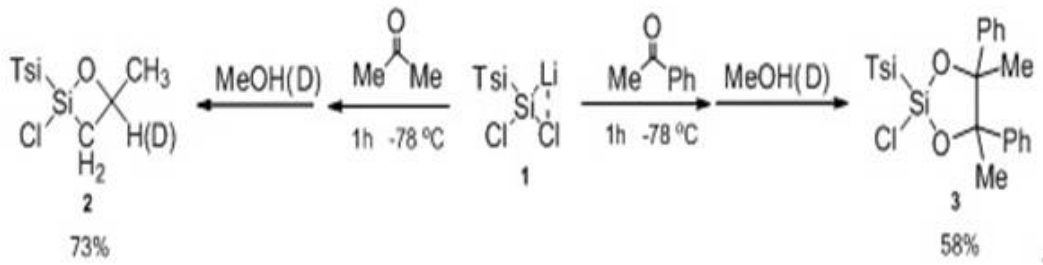
발표종류: 포스터, 발표일시: 금 10:30~12:30

Silylenoid Chemistry: Reactivities of Chlorosilylenoid with Carbonyl compounds

윤수진, 임영묵, 조현모, 이명의

연세대 화학과

Over the past decade, a few novel silylenoids have been the subject of the extensive study. Silylenoid (R_2SiMX) is a compound which has an electropositive metal (M, alkali metal) and a leaving group (X, usually halogen) bound to the same silicon atom. Recently, we reported halosilylenoids, which were stable at room temperature. Chlorosilylenoid 1, having the bulky substituent, Tsi (= trisyl, tris(trimethylsilyl)methyl group), was synthesized by the reduction of trichlorotrisylsilane with 2 equivalent of LiNp (lithium naphtalenide). Using the chlorosilylenoid, 1, we studied its reactivity with various carbonyl compounds, such as acetone, acetophenone, acetaldehyde, benzaldehyde, benzil and β-diketone. After an excess amount of acetone and acetophenone were added to chlorosilylenoid, 1, the treatment of the reaction mixture with an excess of MeOH(D) gave the products, 2-oxasilolane, 2 and 2,5-dioxasilolane, 3, respectively. These results show a novel synthetic application of halosilylenoid as a new route for the synthesis of silaheterocycles.In this presentation, we will discuss the chemistry of chlorosilylenoid with aldehydes as well as ketones.



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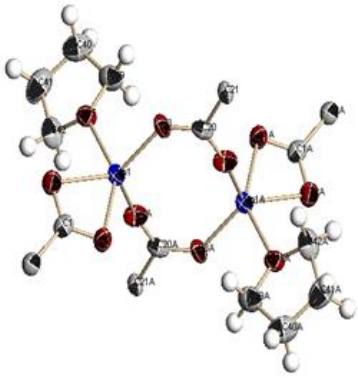
Synthesis and characterization of a Dinulear Manganese(II,II) complex with four terphenyl carboxylate ligands and interaction of water

Sethuraman Kannan, 윤성호

국민대 생명나노화학과

Manganese complexes with carboxylate bridging ligands has evoked considerable interest in the coordination chemistry due to compelling evidence for the presence of a cluster of manganese ions within the oxygen-evolving complex (OEC) of photosystem II (PS II). This Mn_4Ca cluster called the oxygen evolving complex (OEC), is responsible for the light-driven, oxidative coupling of two molecules of water into dioxygen. It is important to establish an artificial OEC model It is important to establish an artificial OEC model not only for understanding and simulating the photosynthetic OEC, but also to construct artificial photosynthesis, which is attracting a great deal of interest to convert solar energy into fuels. Brudvig et al. summarized the preparation, structures, and redox properties of manganese clusters as structural modes of the photosynthetic OEC.Herein, we report the synthesis of neutral bis(μ-carboxylato)dimanganese(II) complex, $[Mn_2(\mu\text{-}O_2CAr^{4F\text{-}Ph})_2(O_2CAr^{4F\text{-}Ph})_2(THF)_2]$ (1) by reaction of $Mn(OTf)_2.2CH_3CN$ and 2,6-di(4-fluorophenyl)benzoate) ($NaO_2CAr^{4F\text{-}Ph}$) in THF. N-donor ligand isoquinoline was introduced into windmill-type dimanganese(II) compound (1), resulting in $[Mn_2(\mu\text{-}O_2CAr^{4F\text{-}Ph})_2(O_2CAr^{4F\text{-}Ph})_2(C_9H_7N)_2]$ (2). Both the compounds have been characterized by X-ray crystallography and IR spectroscopy. Further, attempts are being made to incorporate water molecules into the dimetallic core in both 1 and 2 and also study the electrochemistry of all the complexes. Acknowledgement: This work was supported by the Korea Science and Engineering Foundation(KOSEF) grant (NO. R01-2008-000-11812-0) funded by the Korea government(MEST)



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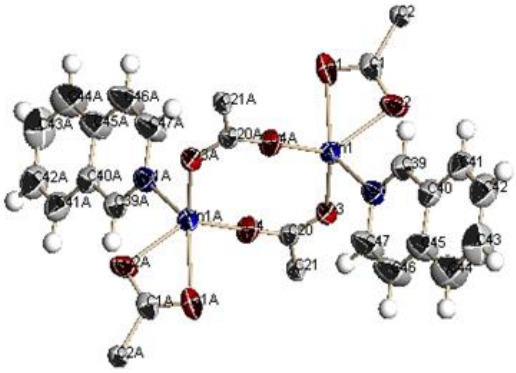

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Acid Catalysis Behavior of Hierarchical Mesoporous ZSM-5 Zeolites

김해련, Eko Adi Prasetyanto, 박상언

인하대 화학과

Mesoporous zeolites are extremely desirable for developing green processes due to their enhanced catalytic performance in comparison to conventional zeolites. The mesopores would help the reactant molecules to access the active sites of zeolies. Microwave synthesis enabled to synthesize hierarchical mesoporous ZSM-5 with sulfonic functionalized ZSM-5 crystals by dual templating method. This mesoporous ZSM-5 possessed both periodic mesoporosity due to the template and crystalline nature of zeolites. However, conventional hydrothermal synthesis resulted in intercrystalline mesoporosity with strong zeolitic crystallinity. The remaining sulfonic ions played role as Bronsted acid sites together with intrinsic zeolitic active sites which contributed to give acid catalytic behaviors. In present work, the role of mesoporosity of three kind of hierarchical mesoporous ZSM-5 (e.a. hierarchical mesoporous ZSM-5 after calcination, extraction, and conventional ZSM-5) were investigated in several acid catalytic reactions such as condensation of acetophenone, esterification of n-octanoic acid with benzyl alcohol, and one pot multi cascade reaction.

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Confinemenet Effect of Encapsulated Chiral Copper(II) Complexes in Zeolite and Mesoporous Zeolite Catalysts for Asymmetric Synthesis of b-Hydroxy Nitroalkanes via Nitroaldol Reaction

Eko Adi Prasetyanto, 김해련, 박상언

인하대 화학과

Chiral copper(II) complexes of secondary bisamines derived from 1,2-diaminocyclohexane were successfully encapsulated into the cavities of zeolite Y and mesoporous ZSM-5 zeolite. These catalysts were characterized by various physicochemical techniques and employed for enantioselective nitroaldol reaction of various aldehydes. Excellent yield (99%) of benzaldehyde with up to 94% enantioselectivity was achieved forming the forming the corresponding b-hydroxy nitroalkanes. In comparison with its homogeneous analogues, the zeolite encapsulated copper complex performed better enantioselectivity. In here we proof that by encapsulation chiral metal complex into zeolites cavities is not only bringing homogeneous reaction to heterogeneous reaction system but also offering other significant benefit that is enhancement of enantioselectivity.

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Synthesis of Highly Fluorescent Fe_2O_3 - CdSe Nanocomposites and Brilliant Blue Photoluminescence (Blue QD)

홍석민, 송릿다, 류지영, 권해진

한국파스퇴르연구소 Nano/Bio Chemistry

Recent advanced in organometallic synthesis have enabled the size and shape dependent preparation of magnetic nanoparticles(MPs), such as Fe2O3, Fe3O4, and FePt MPs(1), and semiconducting quantum dot, such as CdSe/ZnS, CdTe QDs(2), which can be used in a myriad of applications in electronics(3) and biology.(4) Hybrid bifunctional nanoparticles are emerging as useful probes for magnetic based targeting, delivery, cell separation, magnetic resonance imaging(MRI), and fluorescence based biolabeling applications.(5)

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Facile Synthesis of Hexagonal $NaGdF_4$: Yb^{3+}, Er^{3+} (Tm^{3+}) Upconversion Nanoparticles with Magnetic and Luminescent Dual Modality

류지영, 박혜영, 송릿다

한국파스퇴르연구소 Nano/Bio Chemistry

Synthesis of nanomaterials with multi-imaging modality is of great importance in clinical molecular imaging and diagnostics. This study shows novel synthetic strategy to create upconversion nanoparticles with inherent magnetic properties due to Gd in the host material, therefore, having potential to be used as contrast agent in magnetic resonance imaging (MRI). By introducing simple precursors, $NaGdF_4$: Yb^{3+}, Er^{3+} (Tm^{3+}) with pure hexagonal crystalline structure has been created. Nanoparticles doped with Tm^{3+} displayed emission bands extending well to near IR region. Water solubilization of $NaGdF_4$: Yb^{3+}, Er^{3+} (Tm^{3+}) was achieved by coating the nanocrystals with amphiphilic polymer. For biological applications, Ni-Nitrilotriacetate (NiNTA) was employed to test specific biological binding ability. In a model system, NiNTA-$NaGdF_4$: Yb^{3+}, Er^{3+} (Tm^{3+}) showed strong binding to six histidine (6His) modified agarose beads. The $NaGdF_4$: Yb^{3+}, Er^{3+} (Tm^{3+}) nanoparticles exhibit strong upconversion properties and magnetic contrast effect.

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Synthesis of QD-DNA conjugates using NiNTA-Histidine interaction

권해진, 송릿다, 홍석민, 박혜영

한국파스퇴르연구소 Nano/Bio Chemistry

We studied the complexation of QD with DNA using NiNTA-Histidine interaction. In this study, we synthesized 6xHis-tagged QDs and Ni-NTA-modified oligonucleotide. As-synthesized Ni-NTA-modified oligonucleotide was subjected to hybridize with the complementary target BHQ1-tagged DNA. And the complexation of QD with DNA is proved with fluorescence resonance energy transfer techniques. Treatment of the dsDNA-QD complex with imidazole resulted in the cleavage of NiNTA-Histidine interaction and the recovery of the QDs' fluorescence.

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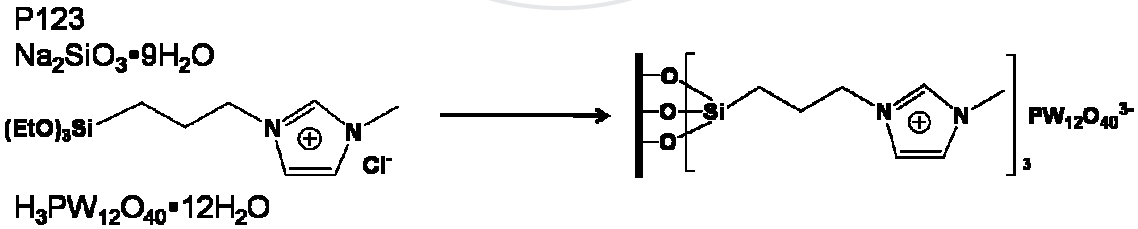
Polyoxometalate(POM) Supported Imidazolium Ionic Liquid-Functionalized SBA-15 as a Heterogeneous Catalyst for Oxidation of Cyclohexene

Jin hua, 박상언

인하대 화학과

Polyoxometalate (POM) have received much attention in catalysis because of their hydrolytic and thermal stability, solubility in various media, tunable acid and redox properties at the molecular or atomic level, and so on.In this work, we immobilized Phosphotungstic acid onto the N-methylimidazolium[Cl-] functionalized SBA-15. The catalytic activity was demonstrated in the oxidation of cyclohexene with 30% aqueous hydrogen peroxide as oxidant at room temperature. The catalyst showed excellent conversion of cyclohexene almost 100% and selectivity of 73% to cyclohexene oxide.



Scheme

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High Photocatalytic Activity of 3,4,9,10-perylenetetracarboxylic diimide Modified Titanium Dioxide Using UV pre-treatment effect

김지원, 김민해, 김희성, 유국현, 김영순

동국대 화학과

Fe_2O_3, Ag_2O, $CaWO_4$ and Gd_2O_2S:Tb loaded on titanium dioxide photocatalysts were prepared by a calcination. And then, 3,4,9,10-perylenetetracarboxylic diimide (PDI) is modified. Specific surface area ratio of 3,4,9,10-perylenetetracarboxylic diimide is 5 ~ 10 % against the TiO_2. Their composite films containing water-born polyurethane used as a material for immobilization were obtained by spray coating technique. The photocatalytic activity of the titanium dioxide films was characterized by decrease of UV-vis absorption spectra for methylene blue and gas chromatography for photocatalytic decomposition of formaldehyde. As a result, photocatalytic activity was increased by metal oxide and 3,4,9,10-perylenetetracarboxylic diimide. It was shown that the Gd_2O_2S:Tb modified titanium dioxide films had best photocatalytic properties. And, photocatalytic activity of TiO_2 using UV pre-treatment effect is better than non UV-pre treatment TiO_2

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N-treatment of mesoporous carbon

모용환, 박상언

인하대 화학과

In industry, they have used to generate energy by using fossil fuels. However, amounts of flue gas have been raised during energy production. CO2 which remain flue gas is one of the problems to global warming. There are three kinds of technology to remove CO2 gas; (1) pre-combustion capture (via oxygen-blown gasification) (e.g. integrated gasification combined cycle technology); (2) oxy-fuel combustion, i.e. removing nitrogen before combustion (e.g. oxy-fuel gas turbine technology); and (3) post combustion capture. Moreover, post combustion capture has advantage such as no washing water, no corrosion, good for high concentration of CO2 gas, and simple design1.Zeolite X13, A4, and Activated carbon were studied to CO2 capture like a post combustion. In volume per gram (cm3/g), activated carbon has higher property of CO2 absorption than zeolite 13X2. The purpose of N-treatment on mesoporous carbon was increasing contents of nitrogen in it. CO2 gas can be easily adsorbed on N-site. Moreover our mesoporous carbon had high surface area and easily went through CO2 gas due to its short channels of hexagonal plate3.Mesoporous carbon was synthesized by amino-functionalized SBA-15 as a hard template in accordance with method in our previous research4. And then it was treated by using HNO3 as an oxidant and was directly reduced by NaBH4 as a reducing agent5. Treated Mesoporous carbon on textural property was studied by scanning electron microscopy (SEM), N2-desorption isotherm, temperature programmed desorption (TPD), thermo gravimetric analysis (TGA), and infrared Fourier transform spectroscopy (FT-IR).

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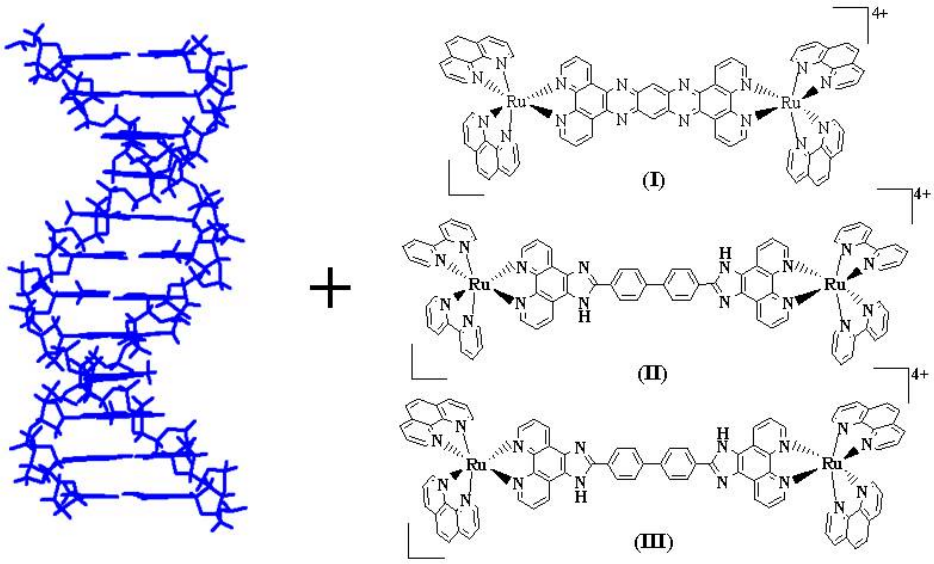
Binding modes of *bis*-Ru(II) complexes with native DNA

프리아, *장윤정, *김석규, **이효선

*경북대 화학과 *영남대 화학과 **경북대 자연과학대학 화학과*

Interaction of Ru(II) complexes that possesses aromatic planar rings with DNA have been a subject of intense studies due to its potential biological applications. Three *bis*-Ru(II) complexes with structurally different bridges and their binding to double stranded native DNA was investigated using isotropic absorption, polarized light spectroscopy including circular and linear dichroism (CD and LD), and fluorescence techniques. The complex (I) exhibited large red-shift and hypochroism in absorption spectrum and negative LD in the bridge absorption as well as DNA absorption region upon binding to DNA. All this observations indicated that the bridge moiety of the complex (I) is parallel to the DNA base plane and supported intercalation binding mode. On the other hand, the complexes (II) and (III) produces LD signal consisting of positive and negative signal in the bridge absorption region and the fluorescence intensity decreased upon binding to DNA although these complexes exhibited red-shift and hypochromism in the absorption spectrum. These contrasting observations indicated that the binding mode of the complexes (II) and (III) is largely deviated from classical intercalative binding. This study demonstrated the importance of the structure of bridging moiety in the intercalation of the *bis*-Ru(II) complex.



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Solvothermal Synthesis of MOF usingtetrakis(4-carboxyphenyl)porphyrin and 4,4'-bipyridine as building block

이승엽, Eko Adi Prasetyanto, 박상언

인하대 화학과

Metal-Organic Frameworks(MOF) are porous crystalline compounds consisting of metal ions or clusters coordinated with rigid organic molecules to form one-, two-, or three-dimensional structures. This MOF could be used for various applications such as hydrogen and carbon dioxide gases storage, gas separation and purification, chemical sensing, drug delivery and catalysis.Here in, we report the preparation and characteristic properties of MOF using 5,10,15,20-tetrakis(4-carboxyphenyl)porphyrin and 4,4'-bipyridine as building block. Solvothermal synthesis with DMF was adopted as an one-pot synthesis of MOF from 5,10,15,20-tetrakis(4-carboxyphenyl)porphyrins, 4,4'-bipyridine and zinc nitrate hexahydrate. This MOF was characterized by Surface area analyzer, X-ray crystallography, Thermogravimetric analysis, etc.

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Microwave Synthesis of Mesoporous ZSM-5 by the Entrapment of Rhodamine-B

MST.NARGIS PARVIN, 박상언

인하대 화학과

Rhodamine B (RB), encapsulated in ZSM-5 zeolites (Si/Al = 50 and Si/Al =30) were successfully synthesized in a one-step sol–gel process under microwave irradiation. The characteristics of RB-ZSM-5 zeolites were investigated using X-ray powder diffraction, Scanning electron microscopy and Nitrogen adsorption-desorption isotherm. Along with the investigation of these characteristics, the acidic properties were also fruitfully characterized by using NH3-TPD profile. The successful incorporation of RB ZSM-5 was confirmed by UV and fluorescence spectroscopy.

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Synthesis and Characterization of Polyethylenes with Triarylamine Side-Groups: Effects of Catalyst Structure and Triarylamine Functionality

박명환, 박준하, 도영규, *이민형

*KAIST 화학과 *울산대 화학과*

Single-site group 4 metallocene catalytic systems have enabled us to produce polyolefins with the tailored polymer architecture in terms of molecular weight, functionalities, and degree of functionalization, which in turn may lead to intriguing properties. Particularly, polyolefins bearing triarylamine (TAA) functionality could be of great interest in display applications like OLEDs since they can possess hole-transporting properties. In this regard, we recently reported that polyethylene bearing triphenylamine group can act as hole-transporting layer materials in OLEDs. As part of our continuous contributions to this area, we have investigated the effects of catalyst structure and triarylamine functionality on the ethylene/a-olefin copolymerization. The details of synthesis, characterization and photophysical properties of polymers will be presented.

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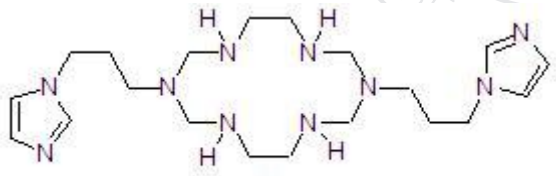
The Structure of Nickel (II) Complex Containing Hexaaza Macrocycles and Carboxylate Ligands

김태형, 김주창

부경대 화학과

One novel complex [Ni(L)(cd)]n (1) (where L = 1,8-di(1-propyl-imidazole)-1,3,6,8,10,13-hexaazacyclotetradecane, cd = cyclohexanedicarboxylate) has been synthesized and structurally characterized by a combination of analytical, spectroscopic and X-ray diffraction methods. The structure shows 1D coordination polymer, in which nickel (II) ions are connected with carboxylate ligands. In the structure of 1, 1D chains are formed by the reaction between [Ni(L)](ClO4)2 and cd. The detailed structure of 1 is discussed in this presentation.



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Aluminum-Salen Complexes as Host Materials for Red Phosphorescent Organic Light-Emitting Diodes

배혜진, 도영규, *이민형

*KAIST 화학과 *울산대 화학과*

The properties of aluminum-salen complex, [salen(3,5-^{t}Bu)H_2Al(OR)], R=OC_6H_4-p-C_6H_6 (H1) and R=[salen(3,5-^{t}Bu)AlOPh]C$(CH_3)_2$ (H2) (salen=N,N´-bis(salicylidene)-ethylenedi amine) as host layer materials in phosphorescent organic light-emitting diodes (PhOLEDs) were investigated. H1 and H2 exhibits high thermal stability with decomposition temperature of 330 and 370 ℃. Both molecules are found to form an amorphous solid with glass transition temperature of 112 and 172℃. Electroluminescence devices based on the vacuum-deposited H1 as a host and Ir(btp_2(acac) (btp = bis(2-(2-benzothienyl)-pyridinato; acac = acetylacetonate) as a red phosphorescent dopant, respectively, display high device performances in terms of brightness, luminous and power efficiencies comparable to those of the device based on a CBP (4,4-bis(N-carbazolyl)biphenyl) host. Details of properties and OLED characteristics of H1 and H2 as host materials will be described.

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Properties of derivated pentacene and photovoltaic device

황윤희, 임이슬, 민선기, 한성환

한양대 화학과

Pentacene that is conjugated molecule becomes already known p-type material, is good packing each molecule and has fast hole mobility.It can be fabricated gas phase deposition because pentacene is not soluble in all organic solvent. Our derivated pentacene has 30 % of hole mobility compared pentacene and it can be dispersed in chloroform, chlorobenzene and so on. In liquid phase, deposited derivated pentacene can be easily, simply and inexpensively applied to solar cell and OLED etc.

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conjugated polymer-sensitized organic-inorganic hybrid solar cell

이미선, 윤석준, 채강일, 한성환

한양대 화학과

We present a method for preparing conjugated polymer-sensitized organic-inorganic hybrid solar cell based on ZnO/CdS/LM-polymer/P3HT/Au using water-soluble acetylene polymer sensitizers(LM2, LM3 polymer). It is important to note that conjugated polymers are generally hydrophobic, whereas inorganic compounds are superhydrophilic (water contact angle< 10°). As a result, the hydrophilicity mismatch causes critical problems for the interfacial contacts. The problem was solved through the hydrophilicity of the polymer was modified toward hydrophobicity by anion exchange. Therefore we can control the character of interface between the hydrophilic material and hydrophobic material.

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발표분야: 무기화학
발표종류: 포스터, 발표일시: 금 10:30~12:30

Carbazolyl based High Extinction Coefficient HMP dyes Designed for Efficient ZnO-based Dye-sensitized Solar Cells

길병호, **Ganesh,** 이덕연, 한성환

한양대 화학과

A photoconductive polymeric molecule, carbazole (HMP11), and electron donating di-substituted triphenyl amine moiety (HMP9) are engineered and compared in ruthenium complex sensitized ZnO solar cell to achieve a remarkable solar to light conversion efficiency of 7.09% and 5.34%, respectively, under a light intensity of 100 mW/cm2. The theoretical iso density surface plots of HMP 9 and HMP 11 calculated from DFT and TDDFT calculations well supports this phenonminal increase in efficiency.

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발표종류: 포스터, 발표일시: 금 10:30~12:30

Three Dimensional CdSe/Single-walled Carbon Nanotubes Solar Cell with Reverse Field-Enhancement Effects

민선기, 한성환

한양대 화학과

The field enhancement phenomenon of SWNTs is utilized to design 3-dimensional (D) CdSe solar cell showing improved performance. In this, fibrous CdSe nanowires were grown onto the SWNTs/ITO surface by electrodeposition, which formed a 3-D solar cell system. The photovoltaic performance study of 3-D CdSe/SWNTs/ITO solar cell showed 3.34% conversion efficiency under AM 1.5 condition (I = 100 mW/cm2), which is significantly higher (50 %) than that without the SWNTs layer. The observed improvement in cell performance is attributed to the reverse field enhancement effects of the SWNTs. Interestingly, the reverse field enhancement factor (β value) of CdSe/SWNTs/ITO is found to increase by 380% with SWNTs layer, wherein texturized Si is used as cathode.

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발표종류: 포스터, 발표일시: 금 10:30~12:30

A Metal–Organic Framework with a Pillared Kagomé Layer Topology

나명수, *Liu Xinfang

*울산과학기술대 친환경에너지공학부 *한양대 응용화학과*

A microporous 3D metal–organic framework with high thermal and hygroscopic stability was prepared by the solvothermal reaction of copper nitrate with a ligand simultaneously containing both a benzenedicarboxylate (bdc) residue for a copper paddle-wheel ($Cu_2(COO)_4$) as a secondary building unit (SBU) and a pyridyl residue as a pillar unit between the SBUs. The 3D framework structure was constructed based on copper paddle-wheels ($Cu_2(COO)_4$) as SBUs in 2D layers of Kagomé topology, which were further pillared by the pendent pyridyl residues of the ligands to form a 3D framework with complicated 3D cavities. The N_2 sorption isotherms of the activated MOF at 77 K showed stepwise adsorption and desorption isotherms with no hysteresis around the step of the low pressure region but with a small hysteresis around the higher pressure region. However, the N_2 sorption of the same activated MOF at 87 K did not indicate any stepwise sorption behaviors but showed type Ⅰ sorption isotherms with less amount of N_2 adsorption.

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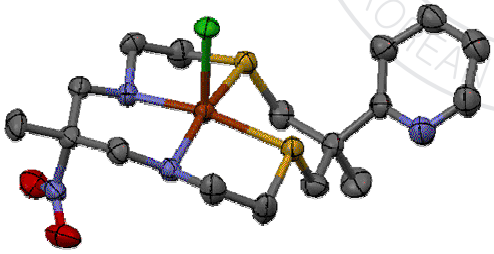
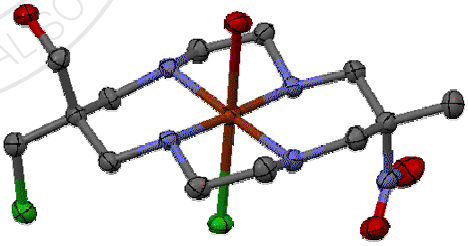
Pendent-Arm Macrocycles Derived from Functionalized Tetradentate Ligands

김미현, *김양, 조정환, **이홍인, *신디, *김향후

*고신대 화학신소재학과 *고신대 화학 신소재학과 **경북대 화학과*

Reaction between ethane-1,2-diamine or 2-aminoethanethiol and 3,3-bis(chloromethyl)oxetane, 2-methyl-2-(pyridin-2-yl)propane-1,3-diyl bis(4-bromobenzenesulfonate) or 2,2-bis(bromomethyl)propane-1,3-diol resulted in tetradentate ligands, which were prepared Cu(II) or Co(III) macrocycles having pyridyl, hydroxymethyl or chloromethyl pendent groups. X-ray crystal structural analyses and EPR spectra of the complexes will be presented.





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발표코드: **Ⅲ33P123포**
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발표종류: 포스터, 발표일시: 금 10:30~12:30

Enantio-selective Sorption between [Zn_2(bdc)(L-lac)(dmf)] and Phenylethanol

서경원, *Dybtsev N. Danil, 김기문

*포항공과대 화학과 *포항공과대 첨단재료과학부*

Homochiral metal-organic porous materials (MOPMs) built from transition-metal ions and chiral ligands are promising materials for enantioselective sorption and separation of chiral molecules. Nevertheless, the number of reports of stereoselective sorption in the homochiral MOPMs is still limited. Here we present the enantioselective sorption of racemic alcohols using zinc(II) lactate-terephthalate [Zn_2(bdc)(L-lac)(dmf)] (bdc = benzenedicarboxylic acid, L-lac = L-lactic acid, dmf = dimethylformamide), characterized by DSC, HPLC and optical rotation methods. Moreover, we obtain single-crystal x-ray diffraction data for comprehensive understanding of the nature of host guest interactions and chiral recognition.

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Cyanide bridged thulium-Group VIII transition metals heterobimetallic complexes arrays {(DMF)10Tm2[M(CN)4]3}∞

송민아, 하성인, *문상봉, **정장훈

*명지대 화학과 *엘켐텍 **명지대 자연과학대학/화학과*

Cyanide briged lanthanide metal thulium-group VIII transition metals heterobimetallic thulium-transition metal complex {(DMF)10Tm2[M(CN)4]3}∞ (M = Ni, Pd, Pt) was quantitatively prepared in metathesis reaction of 2:3 molar ratio of TmCl3 with K2M(CN)4 (M = Ni, Pd, Pt) in DMF at room temperature. The structure of the complex was shown to possess the general formula {(DMF)10Tm2[M(CN)4]3}∞ (M = Ni, Pd, Pt) with one dimensional array, based on single-crystal X-ray analysis. Tm (III) ions in the complex are bridged by the bidentate M(CN)4 2- anions and the repeating unit of the complex is translated only along the crystallographic a axis of the lattice. The structure consists of two parallel running zigzag chains that are inverted from each other. {(DMF)10Tm2[M(CN)4]3}∞ (M = Pd, Pt) complexes are generated by two M(CN)42- ions bridging Tm(III) ions in trans fashion. However, {(DMF)10Tm2[Ni(CN)4]3}∞ complex is generated by two Ni(CN)42- ions bridging Tm(III) ions in cis fashion.

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Conformational Preferences of X-Pro Sequences: Ala-Pro and Aib-Pro Motifs

변병진, 강영기

충북대 화학과

Conformational preferences and prolyl cis-trans isomerizations of the X-Pro motifs (Ac-X-Pro-NHMe, X = Ala and Aib) are explored using the meta-hybrid functional M06-2X and the double-hybrid functional B2PLYP-D with empirical dispersion corrections in the gas phase and in water, where solvation free energies were calculated using the implicit SMD model. Ac-Ala-Pro-NHMe favors the type VI β-turns in the gas phase and the open conformations in water. The populations of type VI β-turns decrease from 71% in the gas phase to 21% in water, which is reasonably consistent with IR and NMR experimental results on *t*Boc-Ala-Pro-NHMe. However, Ac-Aib-Pro-NHMe prefers the type I β-turns with α-helical structures for both residues in the gas phase and in water, whose populations are estimated to be 66% both in the phases. These calculated results may rationalize the reason why most of the peptaibiotics containing the Aib-Pro sequence have a regular α-helical conformation at the N- or C-terminus but a kinked α-helical structure in the middle of the helix. The cis-trans isomerizations of the Ala-Pro and Aib-Pro peptide bonds proceed via the clockwise rotation with the different backbone conformations. The rotational barriers to cis-to-trans isomerization are estimated to be 19.73 kcal/mol for the Ala-Pro tripeptide and 16.64 kcal/mol for the Aib-Pro tripeptide in water, which indicates that the rotational barrier becomes lower by ~3 kcal/mol for the Aib-Pro peptide bond. The calculated rotational barrier for Ac-Ala-Pro-NHMe is consistent with the observed value of 19.3 kcal/mol for Suc-Ala-Ala-Pro-Phe-pNA from NMR experiments in a buffered solution.

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발표종류: 포스터, 발표일시: 목 10:30~12:30

Reaction Mechanism Studies of 2,2,2-Trichloro-1,1-Dimethylethyl Chloroformate

고한중

전주교육대 과학교육과

The specific rates of solvolyses of 2,2,2-trichloro-1,1-dimethylethyl chloroformate in 33 solvents can be well correlated using the extended Grunwald-Winstein equation, with incorporation of the NT solvent nucleophilicity scale and the YCl solvent ionizing scale, with sensitivities towards changes in the scale having values of 1.42±0.09 for l and 0.39±0.05 for m, respectively. The activation enthalpies are ΔH = 12.3 to 14.5 kcal/mol and the activation entropies are -28.2 to -35.5 cal·/mol·K, consistent with the proposed bimolecular reaction mechanism. The kinetic solvent isotope effect of 2.14 in MeOH/MeOD is in accord with a bimolecular mechanism, probably assisted by general-base catalysis.

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발표종류: 포스터, 발표일시: 목 10:30~12:30

Accumulated Proton-Donating Ability of Hydrogen-Bonded Solvent Molecules in Proton Transfer

박선영, 장두전

서울대 화학부

Solvent-inventory experiments on the excited-state proton transfer of a 7-hydroxyquinoline molecule complexed cyclically with two alcohol molecules in the host medium of n-alkane have been carried out with various combinations of alcohols having different proton-donating abilities. The protontaion, which is the rate-determining step, of the imino group of 7-hydroxyquinoline by an alcohol molecule hydrogen-bonded directrly to the imino group initicates the proton-transfer reaction, and subsequent deprotonation of the enolic group completes the reaction without producing any reaction intermideate. Two alcohol molecules participating in the hydrogen-bonded chain of the cyclic complex accelerate proton transfer in a concerted fashion by accumulating their proton-donating abilities. At the rate-determining step, the deprotonation of an alcohol molecule adjacent to the imino group is stimulated by the push-ahead effect of the next alcohol molecule from the backside along the proton-transfer pathway. The strength of the push-ahead effect increases with a gap between the proton-donating abiliteis of two alcohols in a combination and decreases with the viscosity of a host n-alkane medium.

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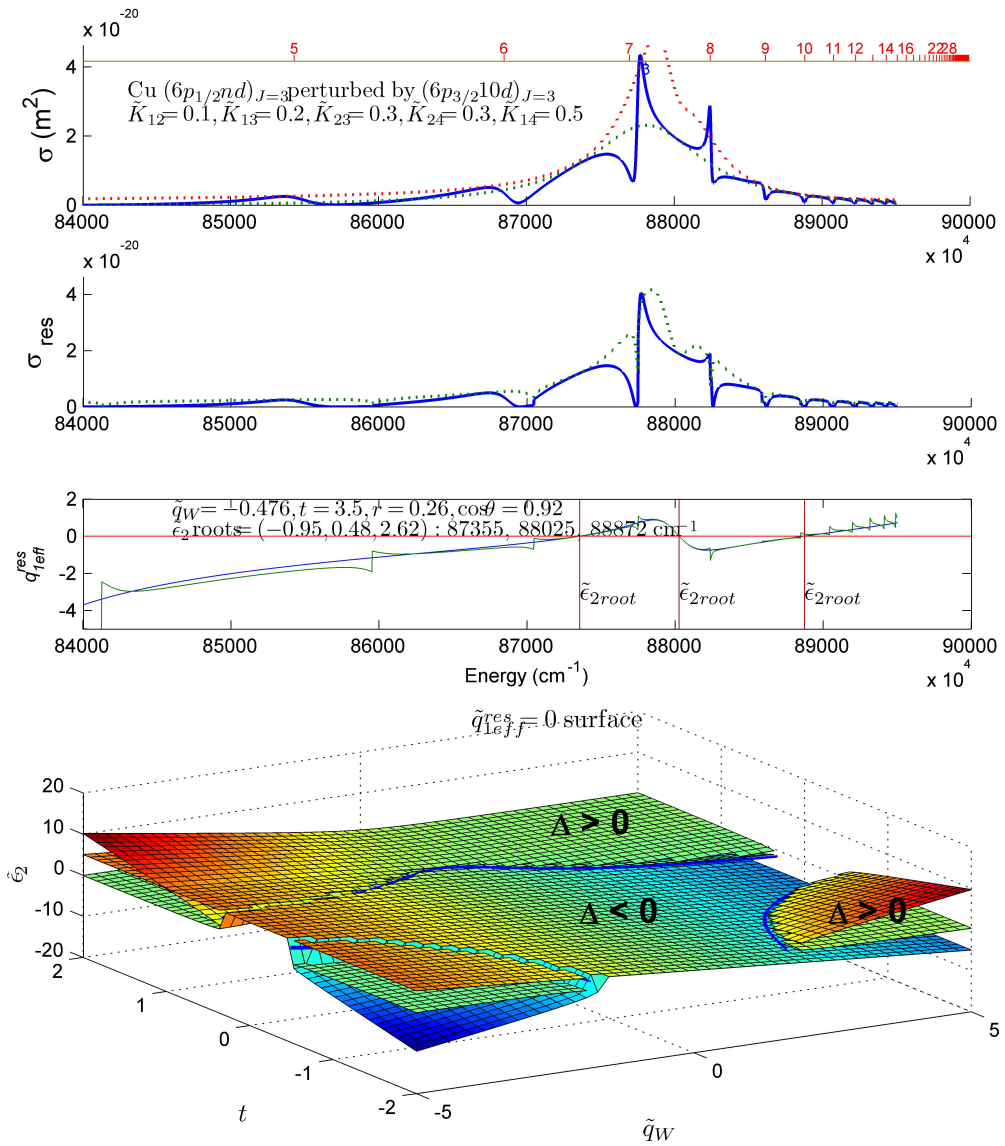
발표종류: 포스터, 발표일시: 목 10:30~12:30

Multichannel quantum defect study of the perturber's effect on the overlapping resonances in Rydberg series for the systems involving 2 closed and many open channels

이천우

아주대 화학과

Martins and Zimmermann's strange-looking photoionization spectra of the Rydberg series (=16-20) perturbed by the interloper provides and interesting application to the present theory. Cohen's 4 channel QDT badly failed for this system since in the spectrum the direct interaction between the closed channels was negligible to the indirect interaction via open channel 3 where his theory cannot be applied. In contrast to his theory, the present theory can be applied to the spectrum, even enjoying two kinds of simplifications, negligible direct interaction between the closed channels and the negligible transition to open channels, not available in other systems. The second simplification available in their spectra is a generic feature of a wide class of experiments known as the isolated core excitations (ICE). Thus the theory developed for their spectra could be also applied to the ICE spectra. The second simplification provides the zero surfaces of in the parameter space of and which can be used as a map to find the route from the starting spectra to the desired one. Depending on the parameter ranges, zero surfaces can be one of among 1, 3, or 1+double root surfaces.


Cu $(6p_{1/2}nd)_{J=3}$ perturbed by $(6p_{3/2}10d)_{J=3}$
$\tilde{K}_{12}=0.1, \tilde{K}_{13}=0.2, \tilde{K}_{23}=0.3, \tilde{K}_{24}=0.3, \tilde{K}_{14}=0.5$
σ (m^2)
σ_{res}
$\tilde{q}_W=-0.476, t=3.5, r=0.26, \cos\theta=0.92$
$\tilde{\epsilon}_2$ roots $=(-0.95, 0.48, 2.62)$: 87355, 88025, 88872 cm^{-1}
$\tilde{\epsilon}_{2root}$
q^{res}_{1eff}
Energy (cm^{-1})

$\tilde{q}^{res}_{1eff}=0$ surface
$\Delta > 0$
$\Delta < 0$
$\Delta > 0$
$\tilde{\epsilon}_2$
t
$\tilde{q}_W$

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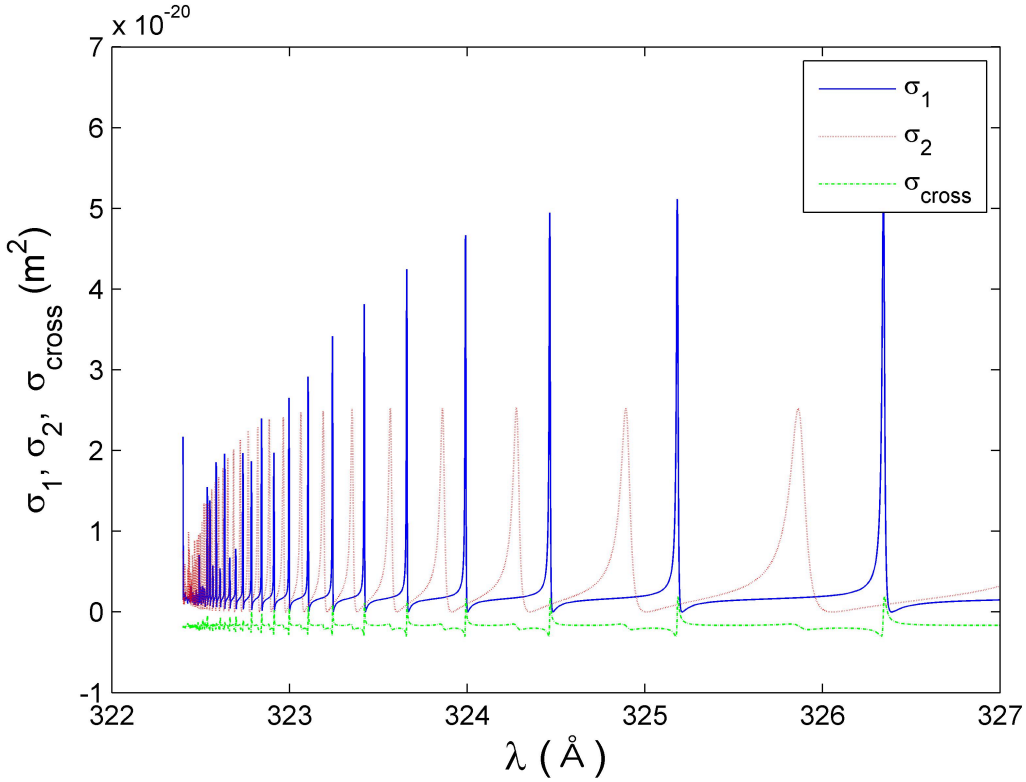
Isolation of resonances in photoionization spectra and time-delay spectra in overlapping sonances for systems involving 1 open and 2 degenerate closed channels

이천우

아주대 화학과

광이온화 스펙트럼은 공명간의 중첩때문에 매우 복잡한 양상을 보이고, 개개의 공명을 분리하는 것은 쉬운 일이 아니다. 본인은 이전에 여러 열린 채널과 중첩된 (같은 이온화 문턱에너지로 수렴) 여러 닫힌 채널이 스펙트럼에 관여하는 계에 대해 시간 지연 스펙트럼에서 이들을 분리해내는 작업이 condiagonalization 이라는 수학적 기법을 씀으로써 이루어질 수 있는 것을 보였고 이를 불활성 기체의 스펙트럼에 적용하였었다. 그런데 이러한 방법을 시간 지연 스펙트럼뿐 아니라 photoionization 스펙트럼에서 분리하는 것은 매우 어려운 일이라는 것이 그 후 연구에서 밝혀졌다. 따라서 이를 좀 더 분명히 하기 위해 우선 관여하는 채널 수를 하나의 열린 채널과 같은 이온화 문턱에너지로 수렴하는 두개의 닫힌 채널이 관여하는 계로 이론을 한정시켜 이러한 문제를 분명히 하였고 이를 Na 에서 s 와 d 두 series 가 $2p^5 3s\ (^1P_1)$ 로 수렴하는 영역에서의 광이온화 스펙트럼에 적용하여 이들을 분리하였다.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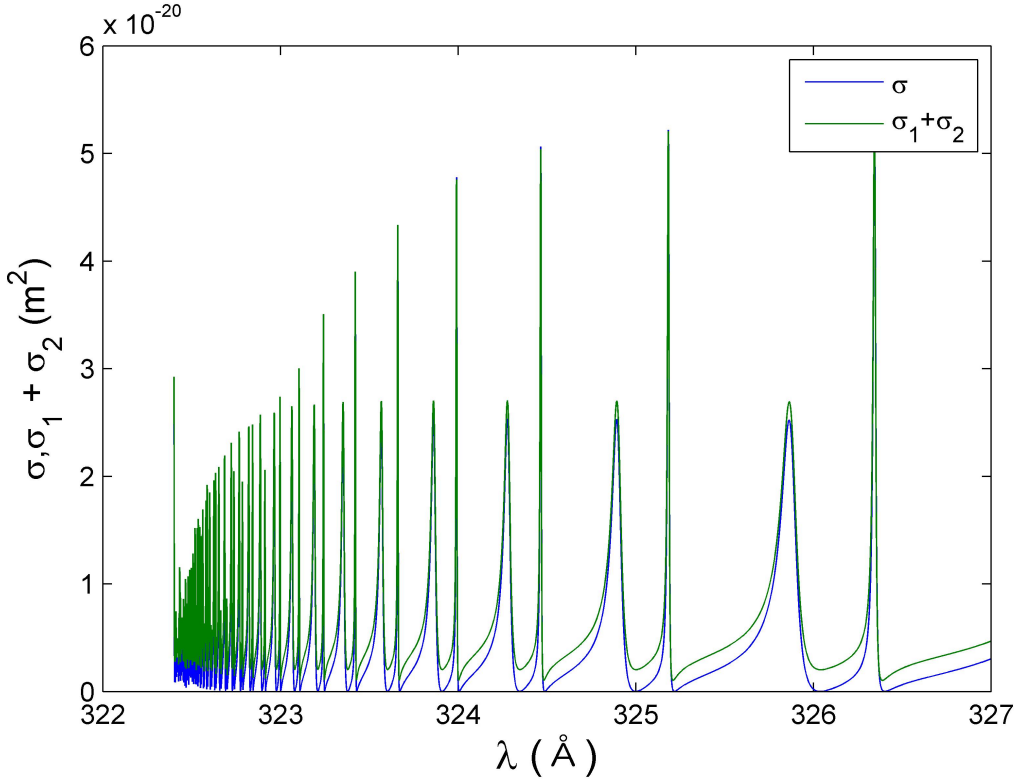
7
6
5
4
3
2
1
0
-1
322
323
324
325
326
327
λ (Å)
σ1, σ2, σcross (m2)
σ1
σ2
σcross


x 10^-20
6
5
4
3
2
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323
324
325
326
327
λ (Å)
σ,σ1 + σ2 (m2)
σ
σ1+σ2

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THE KOREAN CHEMICAL SOCIETY

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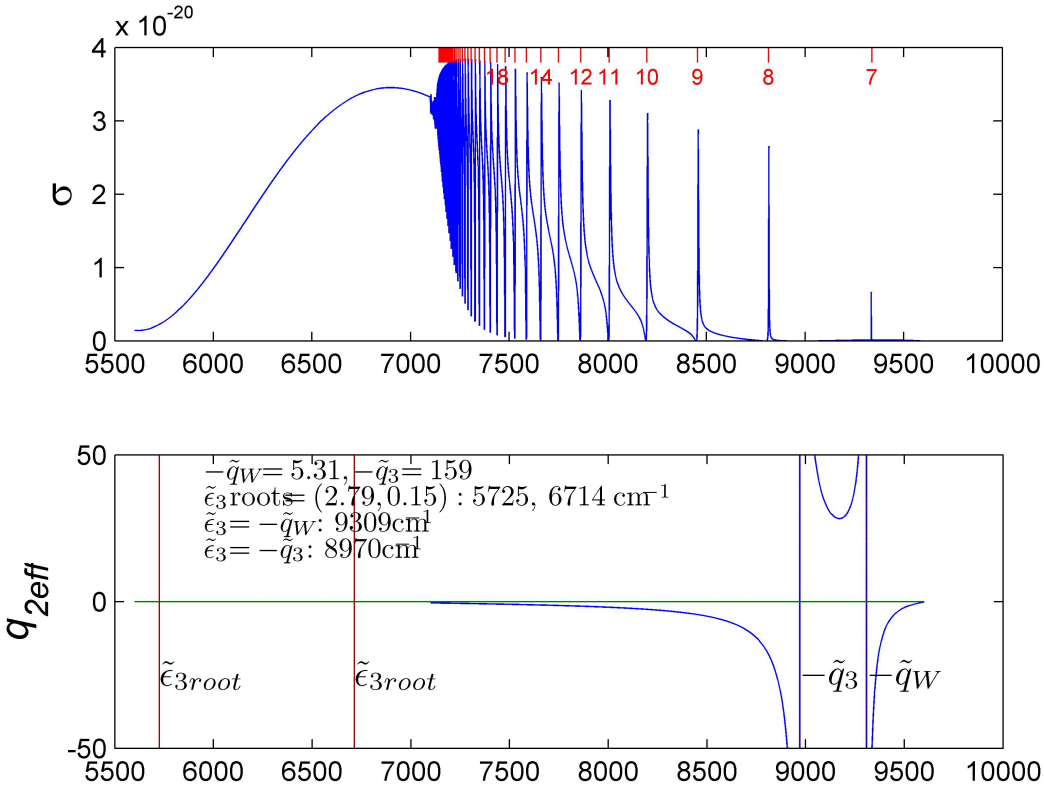
Analytical continuation in line profiles, resonance widths, photoionization cross sections across the threshold for the systems from 1 open, 2 closed channels to 2 open, 1 closed channels

이천우

아주대 화학과

Analytical continuation across the second ionization threshold was specialized for the phase-shifted MQDT system. Formulation for the analytical continuation in line profiles, resonance widths, photoionization cross sections across the threshold for the systems from 1 open, 2 closed channels to 2 open, 1 closed channels was derived, which complements the Gailitis's study on the continuation in autoionization cross sections across the threshold. The connection formula for the line profile index was found to take a particularly simple form when the mutual interaction between closed channels is null.



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Aspect Ratios Modification of Gold Nanorods in Reduction-Limited Conditions

김종엽, *아칠성, 장두전

*서울대 화학부 *한국전자통신연구원 IT융합부품연구소 나노바이오전자소자팀*

Aspect ratios of gold nanorods have been finely modified in reduction-limited conditions via two electrochemical ways: by changing the amount of a growth solution containing small gold clusters in the presence of already prepared gold nanorods as seeds or by changing electrolysis time in the presence or absence of a silver plate. While the atomic molar ratio of gold in the growth solution to gold in the seed solution is critical in the former method, the relative molar ratio of gold ions to silver ions in the electrolytic solution is important in the latter way for the control of the aspect ratios of gold nanorods. The aspect ratios of gold nanorods decrease with an increase of electrolysis time in the absence of a silver plate, but they increase with an increase of electrolysis time in the presence of a silver plate.

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Double Proton Transfer of Excited 7-Azaindole Dimers in a Low-Temperature Organic Glass

임형택, 박선영, 장두전

서울대 화학부

The excited-state double proton transfer of model base pairs, 7-azaindole dimers, is explored in a low-temperature organic glass of *n*-dodecane using picosecond time-resolved fluorescence spectroscopy. Reaction mechanisms are found to depend on the conformations of 7-azaindole dimers at the moment of excitation: planar conformers undergo double proton transfer rapidly in the concerted manner to form tautomeric dimers without forming any intermediate species whereas twisted conformers produce zwitterionic intermediate species rapidly first in the stepwise manner. While the intermediate species transforms into the tautomeric species within 250 ps at 8 K, its reverse reaction also takes place on the time scale of 700 ps. The proton transfer of the intermediate species is almost isotope-independent at cryogenic temperatures because precursor-configurational optimization for intrinsic proton transfer via tunneling is the rate-determining step of the overall proton transfer.

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Excited-State Intramolecular Proton-Transfer-Induced Electron Transfer of Polyquinoline

정혁, 박선영, *유현웅, **박수영, 장두전

*서울대 화학부 *한국표준과학연구원 전략기술연구부 **서울대 재료공학부*

The excited-state intramolecular proton-transfer-induced electron transfer of semirigid polyquinoline is explored in 1,1,2,2-tetrachloroethane (TCE) and *N*-methyl-2-pyrrolidinone (MP) using picosecond time-resolved fluorescence spectroscopy. Reaction mechanisms are found to depend on the rotational conformations of polyquinoline at the moment of excitation: Whereas the trans enolic form does not undergo intramolecular proton transfer within its excited-state lifetime, the cis enolic form does within 15 ps to form a tautomeric zwitterion species. While the subsequent intramolecular electron transfer of the zwitterionic species to yield a tautomeric keto species takes place on the time scale of 25 ps in TCE and 62 ps in MP, its reverse reaction is also followed on the time scale of 28 ps in TCE and 20 ps in MP. No kinetic isotope effects in both of the forward and the reverse electron rearrangement reactions support our proposed mechanisms.

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Fabrication of Copper Oxide Nanoboxes Containing a Platinum Nanocluster via an Optical and Galvanic Route

김미란, 장두전

서울대 화학부

Copper oxide has been of considerable interest because it is a promising material for solar cells and lithium-ion batteries. We report that copper oxide hollow nanoboxes containing a platinum nanocluster have been fabricated in a mild condition at room temperature by dropping a laser-irradiated aqueous platinum colloidal solution on a copper substrate. The irradiation of laser pulses at 1064 nm induced to eject photoelectrons from platinum nanoclusters suspended in water. The aqueous colloidal solution containing photo-oxidized platinum nanoclusters was then dropped on a bulk copper substrate to form hollow $(CuO)_{0.75}(Cu_2O)_{0.25}$ nanoboxes having an average edge size of 195 nm and an average wall thickness of 26 nm, and the resulting platinum nanoclusters, produced by galvanic reduction, remained inside the newly formed copper oxide nanoboxes.

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Composition Variation and Thermal Treatment of $Zn_xCd_{1-x}S$ Alloy Nanoparticles to Exhibit Controlled and Efficient Luminescence

김미란, 박선영, 김재훈, 장두전

서울대 화학부

Alloy nanocrystals are increasingly important in many areas of nanoscale engineering because of the continuous tunableness of their physical and optical properties through the gradual variation of their composition. $Zn_xCd_{1-x}S$ ($0 \leq x \leq 1$) alloy nanoparticles have been fabricated facilely using ethylenediamine as a solvent-coordinating molecular template in water. $Zn_xCd_{1-x}S$ alloy nanoparticles of single-crystalline wurtzite structures having no staking faults have been constructed homogeneously to show that they are intermediate between ZnS and CdS in d-spacing and 2Θ values. The photoluminescence of $Zn_xCd_{1-x}S$ alloy nanoparticles shifts largely to the blue with the composition increase of Zn to have the shortest wavelength at x = 0.9 (λ_{max} = 480 nm for CdS, 396 nm for $Zn_{0.9}Cd_{0.1}S$, 424 nm for ZnS). The thermal treatment of as-prepared $Zn_xCd_{1-x}S$ alloy nanoparticles at 120 ℃ for 10 h has been found to increase photoluminescence intensity and lifetime by a factor of five. This increase has been attributed to the decomposition of coordinated water molecules during annealing processes.

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Substituent Effect on Electron Affinity, Gas-phase Basicity, and Structure of Monosubstituted Propargyl Radicals and Their Anions : A Theoretical Study

이갑용, *권혁재, **송영대

*대구가톨릭대 생명화학과 *대구가톨릭대 화학과 **경운대 한방자원학부*

The substituent effect of electron-withdrawing groups on electron affinity and gas-phase basicity has been investigated for substituted propargyl radicals and their corresponding anions. It is shown that when a hydrogen of the α-CH_2 group or acetylenic CH in the propargyl system is substituted by an electron-withdrawing substituent, electron affinity increases, whereas gas-phase basicity decreases. The calculated electron affinities are 0.95 eV(CH≡C−CH_2•), 1.15 eV(CH≡C−CHF•), 1.38 eV(CH≡C−CHCl•), 1.48 eV(CH≡C−CHBr•) for the isomers with terminal CH and 1.66 eV(CF≡C−CH_2•), 1.70 eV(CCl≡C−CH_2•), 1.86 eV(CBr≡C−CH_2•) for the isomers with terminal CX at B3LYP level. The calculated gas-phase basicities for their anions are 378.4 kcal/mol(CH≡C−CH_2:-), 371.6 kcal/mol(CH≡C−CHF:-), 365.1kcal/mol(CH≡C−CHCl:-), 363.5 kcal/mol(CH≡C−CHBr:-) for the isomers with terminal CH and 362.6 kcal/mol(CF≡C−CH_2:-), 360.4 kcal/mol(CCl≡C−CH_2:-), 356.3 kcal/mol(CBr≡C−CH_2:-) for the isomers with terminal CX at B3LYP level. It is concluded that the larger the magnitude of electron-withdrawing, the greater is the electron affinity of radical and the smaller is the gas-phase basicity of its anion. This tendency of the electron affinities and gas-phase bacisities is greater in isomers with the terminal CX than isomers with the terminal CH.

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Paramagnetic ultrasmall gadolinium oxide nanoparticles as advanced T1 MRI contrast agent

박자영, *백명주, Kattel Krishna, Xu Wenlong, 이강호

*경북대 화학과 *경북대 나노과학기술학과*

We prepared gadolinium oxide nanoparticle for MR contrast agents. Paramagnetic ultrasmall gadolinium oxide (Gd_2O_3) nanoparticles with particle diameters (*d*) of ~1nm were synthesized by using three kinds of Gd(III) ion precursors and by refluxing each of them in tripropylene glycol under an O_2 flow. We characterized them by using HRTEM, TGA, FTIR, cytotoxicity test and MRI instrument. A large longitudinal relaxivity (r_1) of water proton of $9.9 s^{-1} mM^{-1}$ was estimated. As a result, high contrast in vivo T_1 MR images of the brain tumor of a rat were observed.

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Adsorption and Aggregation Characteristics of Ag Nanoparticles onto a Poly(4-vinylpyridine) Film: A Comparison with Au Nanoparticles

류현우, *신권수, 김관

*서울대 화학부 *숭실대 화학과*

The adsorption and aggregation processes of Ag nanoparticles versus Au nanoparticles onto a poly(4-vinylpyridine) (P4VP) surface has been investigated by means of quartz crystal microbalance (QCM), atomic force microscopy (AFM), and Raman scattering spectroscopy. Both the QCM and AFM data indicated that the citrate-reduced Ag and Au nanoparticles are adsorbed onto P4VP, forming only ~33% and ~17% of surface coverage, respectively, even after 6 h of adsorption in solution. The P4VP film was too thin to observe its normal Raman spectrum, but the Raman peaks of P4VP could be detected upon the adsorption of Ag (or Au) nanoparticles onto the film, due to the surface-enhanced Raman scattering (SERS) effect associated with the localized surface plasmon of Ag (or Au) nanoparticles. When in contact with the solution of Ag (or Au) nanoparticles, the SERS peaks of P4VP thus increased linearly as a function of time, in a manner similar to that shown by the QCM and AFM data. As the sol solution was drained off, the SERS signal of P4VP was intensified twice due to the formation of nanoaggregates, and finally the Raman signal induced by Ag nanoaggregates was two times more intense than that induced by Au nanoaggregates, suggesting that Ag nanoparticles must be more advantageous than Au nanoparticles in elucidating by SERS the physicochemical characteristics of organic/polymeric surfaces, including the metal staining in immunoassays and biomolecular sensing.

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Surface Potential of Au Nanoparticles Affected by Layer-by-Layer Deposition of Polyelectrolytes: A Surface-Enhanced Raman Scattering Study

이지원, *신권수, 김관

*서울대 화학부 *숭실대 화학과*

We illustrate by surface-enhanced Raman scattering (SERS) how the surface potential of Au nanoparticles is affected by the layer-by-layer (LbL) deposition of polyelectrolytes onto them. For that purpose, 2,6-dimethylphenylisocyanide (2,6-DMPI) was adsorbed on a poly(ethylenimine) (PEI)-capped Au nanoparticle film, and then its Raman spectrum was taken in various conditions. The NC stretching frequency of 2,6-DMPI is observed at 2123 cm^{-1} in its neat state, but at 2174 and 2157 $cm^{-1}$when 2,6-DMPI is adsorbed on pure Au and on PEI-capped Au nanoparticles, respectively. The initial 51 cm^{-1} blue-shift is due to the transfer of antibonding lone-pair electrons from the isocyanide to gold, and the subsequent 17 cm^{-1} red-shift is caused by the electron donation of PEI to the Au nanoparticles. When negatively charged poly(acrylic acid) (PAA) is deposited onto the PEI-capped Au film, the NC stretching frequency of 2,6-DMPI is then shifted to 2164 cm^{-1}. Consulting a separate potential-dependent SERS measurement, this corresponds to a variation of the surface potential of Au nanoparticles from -0.52 V to -0.32 V. The surface potential of Au nanoparticles alternates upon further deposition of PEI and PAA, but the extent of variation gradually diminishes and the surface potential of Au nanoparticles finally attains a plateau value, i.e. -0.41 V, after the deposition of five bilayers of PAA and PEI. In contrast to the surface potential of Au nanoparticles, the zeta potential varies alternately irrespective of the number of LbL depositions.

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Silanization of Ag-Coated Magnetite Particles: An Efficient Route to Fabricate Magnetic Raman barcoding Materials

최정용, *신권수, 김관

*서울대 화학부 *숭실대 화학과*

In this work, we demonstrate that Ag-coated magnetic particles can be used as core materials for constructing not only the molecular sensing/recognition units but also the barcoding systems both of which operating via SERS. Initially, superparamagnetic magnetite particles with a mean diameter of 400 nm are prepared, and then and then SERS-active silver was coated onto them via a very simple electroless-plating method. One difficulty in the latter application is the necessity of the stabilization of SERS marker molecules adsorbed on Ag particles. The fabrication of silica shells would then be an effective strategy to protect SERS marker molecules. The Raman markers were subsequently assembled onto the Ag-coated silica beads, after which they were brought to stabilization by silanization via a biomimetic process in which poly(allylamine hydrochlorise) layer formed on Raman markers by a layer-by-layer deposition method acted as scaffolds for guiding silicification. Since the proposed method is cost-effective and is suitable for mass production, it is expected to play a significant role especially in the development of SERS-based barcoding devices.

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Silver-Coated Dye-Embedded Silica Beads Applicable as Core materials of Dual Tagging Sensors Operating via Fluorescence and SERS

이향봉, *신권수, 김관

*서울대 화학부 *숭실대 화학과*

We have developed a new type of dual-tag sensors, operating via both fluorescence and surface-enhanced Raman scattering (SERS), for immunoassays. Initially, dye-embedded silica beads were prepared, and then SERS-active silver was coated onto them via a very simple electroless-plating method. The Raman markers were subsequently assembled onto the Ag-coated silica beads, after which they were brought to stabilization by silanization via a biomimetic process in which poly(allylamine hydrochlorise) layer formed on Raman markers by a layer-by-layer deposition method acted as scaffolds for guiding silicification. In the final stage, the dual-tagging sensors were assembled onto them with specific antibodies (antihuman-IgG or antirabbit-IgG) to detect target antigens (human-IgG or rabbit-IgG). The fluorescence signal of the embedded dye was used as an immediate indicator of molecular recognition, while the SERS signals were subsequently used as the signature of specific molecular interactions. The antibody-grafted particles were able to recognize antigens down to 10^{-10}g mL^{-1} solely by the SERS peaks of the Raman markers. For this reason, these materials should find wide application, especially in the areas of biological sensing and recognition that rely heavily on optical and spectroscopic properties.

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The PEG diacid modified gadolinium oxide nanoparticles for T1 MRI contrast agent

백명주, *박자영, *Xu Wenlong, *Kattel Krishna, *이강호

*경북대 나노과학기술학과 *경북대 화학과*

We synthesized paramagnetic ultrasmall gadolinium oxide (Gd_2O_3) nanoparticles by using six kinds of Gd(III) ion precursors; $Gd(NO_3)_3$•$6H_2O$, $(C_2H_3O_2)_3Gd$•xH_2O, $(C_5H_8O_2)_3Gd$•xH_2O, $GdBr_3$•xH_2O, $Gd_2(C_2O_4)_3$•xH_2O and $GdCl_3$•xH_2O. Note that the Gd(III) ion itself has been known to be the best metal ion in the periodic table which can be used as a T1 MRI contrast agent. First of all, it possesses seven unpaired 4f electrons, giving a large electron magnetic moment. No other metal ions possess unpaired electrons more than this. Furthermore, these electrons solely yield the S state electron magnetic moment, and thus, the Gd(III) ion can very efficiently induce the longitudinal relaxation of a water proton. The gadolinium oxide (Gd_2O_3) nanoparticles have been synthesized through several steps by refluxing each of them in triethylene glycol under an O2 flow and coating with biocompatible PEG diacid. And then we characterized them through HR-TEM, XRD, FT-IR, TGA, Squid magnetometer, and MRI instrument.

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Synthesis and Characterization of Lanthanide Oxide Nanoparticles

Kattel Krishna, 박자영, **Xu Wenlong**, *백명주, 이강호

*경북대 화학과 *경북대 나노과학기술학과*

In this work, we described a chemical approach for the synthesis of Eu_2O_3, Dy_2O_3, Er_2O_3 and Ho_2O_3 nanoparticles and characterized them by using HRTEM, XRD, SQUID Magnetometer and MRI instrument. We are also planning to synthesize and characterize some other ultra-fine and monodisperse rare-earth oxide (Ln_2O_3) nanoparticles. The principle aim of our research is for biomedical application of the prepared nanoparticles especially for MRI contrast agent.

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Magnetic and Relaxivity Properties of GdEu oxide nanoparticles

Xu Wenlong, 박자영, **Kattel Krishna**, *백명주, 이강호

*경북대 화학과 *경북대 나노과학기술학과*

Polyethylene glycol diacid (PEG)-surface modified GdEu oxide nanoparticles synthesized in triethylene glycol were nearly monodisperse in diameter and highly water-dispersible. We report a facile one-pot synthesis of GdEu oxide nanoparticles and characterization with XRD, TGA, HRTEM, squid magnetometer, PL spectrometer and MRI instrument. These nanoparticles can be used as MRI contrast agent as well as optical imaging. This dual imaging capability will increase the possibility of an early observation of disease such as cancer.

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The internal twisting motion of an electronically excited hemicyanine dye in viscoelastic media

배은혜, 지아영, 이민영

이화여대 화학나노과학부

The medium influence on the molecular rotor dynamics of trans-4-[4-(dimethylamino)-styryl]-1-methylpyridinium iodide (4-DASPI) in the excited state were investigated in liquids and solids. The twisting rate constants were obtained from the fluorescence quantum yields and lifetimes of 4-DASPI in water-glycerol mixtures and in various polymers. It was observed that condensed phase dynamics of electronically excited 4-DASPI correlate strongly with viscosity and modulus. Therefore, the internal motion of 4-DASPI in viscoelastic media can be explained by the mode coupling effect between the twisting coordinate and medium mechanical property.

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Photoisomerization processes of symmetric cyanine dyes in poly(alkyl methacrylate) polymers

지아영, 박서현, 이민영

이화여대 화학나노과학부

The excited-state twisting motion of 3,3'-diethyloxacarbocyanine iodide (DOCI) and 1,1,'-diethyl-2,2'-cyanine iodide (DCI) were studied in a series of poly(alkyl methacrylate) polymers. The measured fluorescence lifetimes of DOCI and DCI were compared with the glass transition temperature and elastic modulus of polymers, and it was observed that the molecular rotor dynamics of both dyes correlate well with the elastic modulus of the matrix, but with different aspects. The underlying mechanisms are described by the reaction volumes and potential energy surfaces associated with the excited-state motion.

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Elastic modulus mapping of amyloid oligomers and fibrils by fluorescence lifetime imaging

권하늘, 이민영

이화여대 화학나노과학부

The elastic modulus is an important physical property of soft matter, but it is often difficult to attain experimentally. In this work, the elastic modulus of beta-amyloid (Ab) oligomers and fibrils were obtained by fluorescence lifetime imaging microscopy (FLIM). Ab aggregation was known to be a main cause of the pathogenesis of Alzheimer's disease. Ab aggregates were stained with 9-dicyanovinyljulolidine (DCVJ), a rigidity-probing dye, and the fluorescence lifetime distributions were obtained by FLIM. The elastic moduli of Ab oligomers and fibrils were also independently measured by atomic force microscopy (AFM) nanoindentation. Our results indicate that FLIM is a good method for the elastic modulus mapping of soft matter.

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DFT study of small boron cluster isomerization reaction path

장효원

순천대 화학과

Continuing on previous works, transition states are calculated connecting various boron cluster isomers. Several structural building blocks composed of 12 boron atoms are used to form the reacting oligomers. Differences in numerical results are compared obtained by using effective core potential basis and all electron basis.

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Surface Enrichment of Ag Atoms in Au/Ag Alloy Nanoparticles Revealed by Surface Enhanced Raman Scattering of 2,6-Dimethylphenylisocyanide

김경록, *신권수, 김관

*서울대 화학부 *숭실대 화학과*

Surface-enhanced Raman scattering (SERS) of 2,6-dimetylphenylisocyanide (2,6-DMPI) has been investigated using Au/Ag alloy nanoparticles as the adsorbing substrate. UV/vis spectra suggest the formation of alloy nanoparticles is taking place, in conformity with the mole fractions of gold and silver used initially in preparing the alloy sols; according to transmission electron microscopy images, the alloy sols are composed of spherical particles with diameters of ~35 nm irrespective of their composition, from pure Ag to pure Au nanoparticles. We have confirmed that the SERS spectral feature of 2,6-DMPI on pure Ag is distinctly different from that on pure Au. Furthermore, the SERS spectral feature of 2,6-DMPI on Au/Ag alloy particles, even with a nominal composition of 95% Au and 5% Ag ($Au_{0.95}Ag_{0.05}$), is the same as that on pure Ag. The present observation supports our previous contention that the outermost layers of the Au/Ag alloy nanoparticles are highly enriched in Ag atoms compared with their interiors. SERS is thus proven to be an invaluable tool for the surface analysis of alloy metals.

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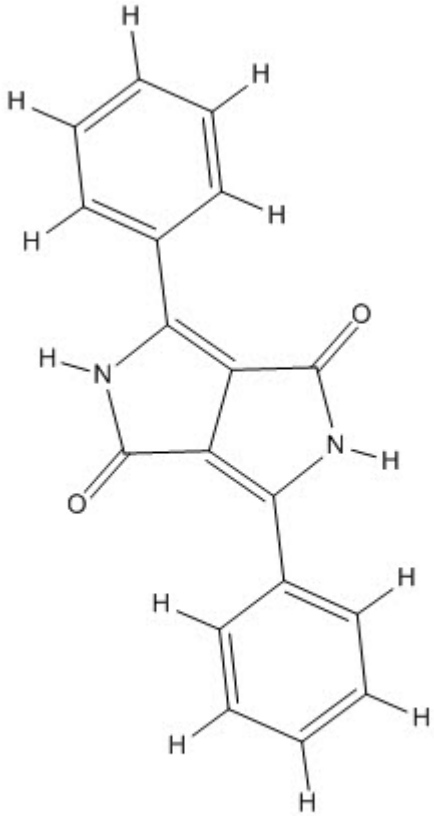
Crystal Structure Prediction studies for the organic pigments : tests on the DPP and DPPP.

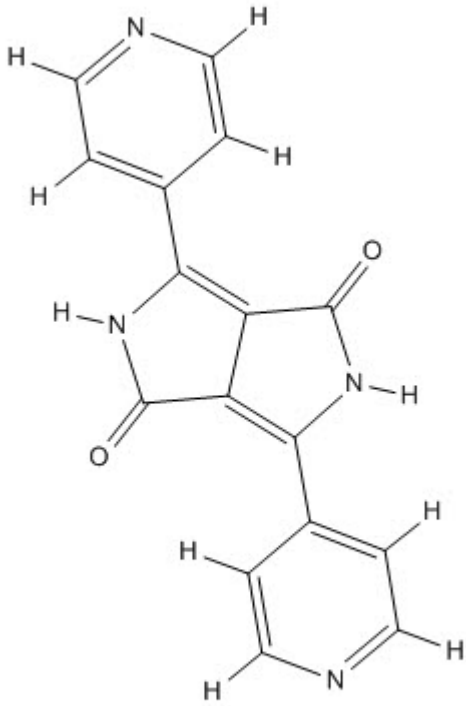
김경현, 김대진, 최승훈, *김용호, 정동현

*(주)인실리코텍 *경희대 화학 및 신소재과학*

지난 10 년간 결정 구조 예측에 관한 다양한 이론과 방법이 발표되었고 이를 검증하고 일반적인 결정구조 예측 방법을 정립하기 위해 Cambridge Crystallographic Data Centre 에서 총 4 회의 blind test 를 수행하였다. 여러가지 방법 들 중 비교적 정확하고 다양한 분자의 결정구조 예측이 가능한 Materials Studio 4.4 의 Polymorph Predictor 모듈과 COMPASS, Dreiding force field 를 사용하여 결정구조 예측을 수행하였다. 결정구조 예측의 대상으로는 최근 EL 과 LCD color filter 의 핵심 안료로 사용되는 붉은색의 1,4-diketo-3,6-diphenylpyrrolo(3,4-c)pyrrole(DPP) 과 DPP 의 유도체로 안료보다는 H_2 gas sensor 로 사용이 가능한 1,4-diketo-3,6-bis(4'-dipyridyl)-pyrrolo-[3,4-c]pyrrole(DPPP)을 이용하였다. 아울러 예측된 결정구조를 X-ray 구조와 비교하기 위해 각각의 구조를 동일 프로그램의 Reflex 모듈을 사용하여 시뮬레이션 된 X-ray Powder Diffraction (XRPD) 데이터를 이용하였다.



(a) DPP



(b) DPPP

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발표분야: 물리화학
발표종류: 포스터, 발표일시: 목 10:30~12:30

The Optical Homogeneity Test of SERS Nanoprobe (SERS Dot^{TM}) for Biomedical Applications

채진주, *김건성, **정대홍

*서울대 과학교육학과 *서울대 사범대 화학교육과 **서울대 화학교육과*

Nowadays, Surface-enhanced Raman Scattering (SERS) is being studied to find its applications as ultra-sensitive biomolecule detection system. Comparing with other labeling agents for biomolecule detection such as enzyme, dye, molecular fluorophore and quantum dot, SERS has the advantages of multiplexing capability, quantification, single laser excitation, photostability and little autofluorescence of cell & tissue by NIR excitation. Among several SERS substrates, SERS Dot^{TM} (1) has been reported to be very stable, sensitive and versatile nanoprobe for biomolecular application because it has stable silica shell, single particle detectability and easiness of functionality introduction such as magnetic(2) or fluorescent(3) property and so on. Because SERS enhancement factor ranges from 10^4 to 10^{14} (4) by the size, shape and chemical composition of metal nanoparticle, it can show inhomogeneous signal and give poor quantification. In this work, as basic research for the quantitative application, we characterized optical properties of SERS Dot^{TM} in respect of signal homogeneity, detection limit and photostability. SERS Dot^{TM} made by the reported procedure(1) was dispersed on Au substrate by covalent bonding. SERS signal of well-separated single SERS Dot^{TM} was collected using LabRam Raman spectrometer using ×100 objective lens and 532 nm excitation of varying laser power. The Homogeneity of SERS signal is analyzed with the relative intensity of the two peaks of Raman label material. Using the property characterized above, now we are trying to realize multiplex quantification of PSA, AFP and CEA by chip-base sandwich assay. References(1) Jong-Ho Kim, et al., Anal. Chem. 2006, 78, 6967-6973 (2) Bong-Hyun Jun, et al., Analytical Biochemistry. 2009, 391, 24-30 (3) Kyeong Nam Yu, et al., Bioconjugate Chem. 2007, 18, 1155-1162(4) Ying Fang, et al., Science, 2008, 321, 388

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Grand Canonical Monte Carlo Simulations for the Hydrogen Uptake on Pillared Covalent Organic Frameworks

김대진, 정동현, 김경현, *최기항, 최승훈

*(주)인실리코텍 *고려대 화학과*

We modeled Pillared covalent organic frameworks (PCOFs) which the “pillar” molecule, pyridine is inserted between the organic layers of COF-1 for the improvement of physisorption ability for the hydrogen molecule. COF-1 is one of the 2D COF (Covalent Organic Framework) and has strong hydrogen adsorption enthalpy but its hydrogen uptake is not so much. Density functional theory (DFT) calculations and grand canonical Monte Carlo (GCMC) simulation were used for the model construction and the prediction of hydrogen uptakes. With this calculation, we proposed new PCOF structures to enhance hydrogen storage capacity both in gravimetric and volumetric unit, 10 ~11 wt% and 59 ~ 63 g L-1 respectively. The increment of hydrogen uptake can be explained in terms of hydrogen adsorption enthalpy and specific surface area. By the insertion of pyridine molecule to elongate the interlayer spcing, the specific surface area increases enough to store the hydrogen molecules and the loss of hydrogen adsorption enthalpy is small.

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Femtosecond Transient Absorption Study for Charge Transfer Dynamics of Gradient Multi-shell Semiconductor Nanocrystals

강준희, *양일승, **장은주, ***전신애, ****장효숙, *****김성근

*서울대 생물물리 및 화학생물학과 *서울대 화학부 **삼성종합기술원 Advanced Materials ***삼성종합기술원 기초소재센터 ****삼성종합기술원 소재기술센터 *****서울대 화학부 & 서울대 생물물리 및 화학생물학과*

The efficiency of semiconductor nanocrystals has recently been greatly improved and they are now widely used in various areas ranging from bio-imaging to light-emitting diodes. Multi-shell semiconductor structure is known to increase the quantum efficiency up to 80% and passivation is reported to strongly enhance its stability. To address these issues from photophysical perspectives, we employed femtosecond transient absorption to investigate the effect of shell thickness and the gradient structure of the multi-shell semiconductor nanocrystals on its charge transfer dynamics.

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Physicochemical Properties of Pulegone in various solvent systems

이호석, *박철호, **박기민, 박형련

*전남대 화학과 *남부대 향장미용학과 **경상대 화학교육과*

Pulegone is a colorless liquid volatile subatance. The substance is contained in a variety of plants such as Schizonepeta tenuifolia. It possesses a characteristic odor and utilizes for the aromatherapy. It is therefore investigated the spectroscopic properties of pulegone in various solvent systems. The substance is soluble in nonpolar solvents. The absorption spectra of pulegone in n-hexane contain two bands, a strong peak at 240 nm and a weak peak at 280nm. The substance emits weak fluorescence. The fluorescence maximum peaks in n-hexane were obtained at 345 nm and 660 nm. Their fluorescence spectra were changed according to the contents of the kinds of solvents. As the polarity of the solvents increased, the fluorescence maximum peaks shifted to a longer wavelength.

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Spectroscopic Properties of Protoporphyrin IX in various solvent systems

이호석, *박철호, **유지봉, ***박기민, 박형련

*전남대 화학과 *남부대 향장미용학과 **경상대 화학과 ***경상대 화학교육과*

Protoporphyrin IX have been attracted considerable attentions to use the substance for the photodynamic therapy of skin tumorsw, because it is able to induce photosensitive reaction in human skin by sunlight. It is therefore investigated the spectroscopic properties of protoporphyrin IX in various solvent systems. The UV absorption spectra of 1.78 X 10-6 M protoporphyrin IX and their fluorescence spectra were changed according to the contents of the kinds of solvents. In polar solvents, The UV absorption spectra show a sharp absorption maximum peak at 408 nm. However, their UV absorbance are measured lower value at the same wavelength in nonpolar solvent. In addition to these, the fluorescence intensities have been also influenced by the polarity of the solvents.

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Structure and Enzymatic Activity of Subtilisin Protein in Organic media

어유진, 함시현

숙명여대 화학과

Structural and dynamical behavior of enzyme is a critical determinant for its catalytic activity. Knowing that the enzyme activity may vary with different solvent polarities due to the changes of its structure and flexibility, Subtilisin Carlsberg enzyme was subjected to investigate the structural variations upon different solvent systems by using quantum mechanics/molecular mechanics (QM/MM) simulations with three different explicit solvent systems. Characterization of the enzyme structure and dynamics in aqueous and in organic solvents is discussed in relation to the solvation of the enzyme active site as well as the role of crystallographic waters around the protein.

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Analysis of Optical Spectral Change of Ag Colloid with Time

진경철, 정대홍

서울대 화학교육과

We oftenly observed temporal UV-Vis spectral change of Ag colloid after production (silver nitrate reduction with sodium borohydride). In this research, the reason of that was investigated by optical measurment, transmission electron microscopy (TEM) and theoretical calculation. The absorption spectra of the colloid showed a shoulder to the red side of main band at the early stage of its production. However, the shoulder became decreased gradually and disappeared in several days. To observe shape evolution of the colloidal nanoparticles, the produced colloid was monitored with transmission electron microscopy (TEM) temporally. It was observed that the initial colloid has more elongated silver nanoparticles than the latter. And the aspect ratio of the nanoparticles was getting less to one as time went on. We also conducted theoretical calculations of the extinction efficiencies, which well agreed with the experimental results, using the discrete dipole approximation (DDA). From these data we can conclude that the temporal UV-Vis spectral change of the Ag colloid is originated from the shape evolution of the silver nanoparticles from ellipsoid to sphere.

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Classical Trajectory Studies of the CH_3 + OH Reaction

김성희, 이종백, *김유항, **H. K. Shin

*전남대 화학교육과 *인하대 물리화학부 **Dept of Chem, University of Nevada, Reno*

The product pathways of the CH_3 + OH reaction have been studied over the temperature range of 300 – 2500 K using classical dynamics procedures for an analytical form of the interaction potential composed of both short-range and long-range terms. The primary step in the reaction is a direct-mode collision between the radicals forming vibrationally excited CH_3OH^*, which either stabilizes to the recombination product CH_3OH or proceeds to form various products (CH_2OH, CH_3O, CH_2O, HCOH, CH_4 and CH_2). The CH_3OH rate constant varies from 3.0×10^{-11} cm^3 $molecule^{-1}$ s^{-1} at 300 K to 7.7×10^{-11} cm^3 $molecule^{-1}$ s^{-1} at 2500 K. At these two temperatures, the reaction cross sections are 3.4 and 3.0 $Å^2$, respectively, showing a slight negative temperature. The CH_3O rate decreases from 6.8×10^{-11} to 6.5×10^{-11} cm^3 $molecule^{-1}$ s^{-1} over the temperature range. The CH_2 rate increases from 1.1×10^{-11} to 1.6×10^{-11}, while the CH_4 rate increases from 5.8×10^{-12} to 7.0×10^{-12}(all in units of cm^3 $molecule^{-1}$ s^{-1}). Of 40 000 trajectories sampled, the numbers of reactive events for CH_2OH, CH_2O and HCOH are less than ten, leading to the rate constants which are in the range of 10^{-14}– $10^{-13}$$cm^3$ $molecule^{-1}$ s^{-1}. For all reaction pathways, the temperature dependence of rate constants is very weak, even showing a negative dependence in some cases, which is typical of the reactions involving free radicals.

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Characteristic of a CNT-Metal Nano-Composite Preconcentrator for GC Analysis of VOCs in Air Samples

이명기

원광대 화학과

Gas chromatographic analysis of complex mixtures of Volatile Organic Compounds (VOCs) encountered in indoor/outdoor working environments has been performed using a small sorption trap preconcentrator. After sample trap by the adsorbent, the flow direction through the preconcentrator is reversed, and the thermally desorbed analyte is directly introduced into the GC capillary column module. Candidate adsorbents, such as CNT-Co, Ni, Co, Al metal nano-composites, were assessed on the basis of thermal-desorption bandwith and enrichment efficiency, chromatographic peak shape, and breakthrough volume against mixture of organic compounds.

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Single Molecule Spectroscopic Investigation of Excimer Dynamics in Cofacial Perylenediimide Dimer and Trimer

유혜진, 김동호

연세대 화학과

π-Stacked perylenediimides (PDIs) have strong electronic communication between the individual molecules and show great promise as organic electronic materials for applications in field effect transistors, photovoltaics and liquid crystal displays. To gain further insight into the relationship between conformational behaviors and electronic structures of π-stacked PDIs, we have investigated changes in the excimer-like state of cofacial PDI oligomers that result from π-stacking in real-time by monitoring the single molecule fluorescence intensity and lifetime trajectories in a PMMA polymer matrix. The fluorescence intensity and lifetime of π-stacked perylenediimides are sensitive to the degree of π-orbital interactions among PDI units, which is strongly associated with molecular conformations in polymer matrix. Furthermore, our results can be applied to probe the conformational motions of biomolecules like proteins.

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Transparent PVC-silicate nanocomposites by interlamellar silylation of layered Ti-silicate: preparation and structural characterization

박경원, 이혜진, 진달샘, 정종화

경상대 화학과

Transparent PVC-silicate nanocomposites were synthesized of Polyvinyl chloride (PVC) intercalation for Octyltriethoxysilane-titanosilicate (OTES-TS). H^+-titanosilicate was modified by interlayer surface silylation using octyltriethoxysilane in ethanol without a pre-swelling step. The organic-inorganic PVC nano-composite membrane was prepared by PVC and (Na^+-titanosilicate), (H^+-titanosilicate), (OTES-TS) were mixed and dissolved in THF. The introduction organic-inorganic PVC nano-composite membrane was confirmed by XRD, RAMAN, SEM, ^{29}Si NMR and TEM as a gallery expander.

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Preparation and characterization of hexagonal shaped nanostructures on Au (111) in UHV

박준범, 유세희, *이국행, *김자홍

*전북대 화학교육 *전북대 화학교육과*

The nanostructure fabrication with energetic ions is a critical tool in the laboratory and industry. The ion-solid collision process at the elevating temperature contains fascinating surface physics, chemistry, and material science. In this presentation, we report fabrication methods of hexagonal shaped nanostructures by using neon and oxygen ion bombardment at different temperature. By adjusting ion energy, flux, and sample temperature, we were able to control the depths and diameters of the nanostructures. The morphology and bonding configurations of the nanostructures were monitored by STM and XPS. Oxygen ion bombardments of Au (111) result in Au-O complex structures, which represent activated gold nanoparticles for CO oxidation reaction and can give a clue to solve their unusual catalytic activities.

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The Study of Aqueous Solution Properties of SDS with PEO in Magnetized Water

이성현, 전상일

강릉대 화학과

자화수(magnetized water)는 원래 물분자가 자화 되어서 자기장의 특성을 갖는다는 의미가 아니라, 자기장에 의하여 물분자 배열이 바뀌어져서 특이한 물의 특성을 보이는 상태를 의미한다. 이전 실험에서 계면활성제의 CMC(critical micelle concentration)는 증류수에서 보다 자화수에서 낮은 농도에서 형성되는 것을 확인하였다. 계면활성제는 용액 속에 소량만 존재하더라도 용액 계면이나 표면의 성질을 바꿀 수 있으며, 농도가 증가함에 따라 세척성, 점성률, 굴절률, 삼투압, 전기전도도, 계면장력 및 표면장력 등이 크게 변화되지만 CMC 를 기준으로 그 이상의 농도에서는 이런 물성들이 크게 변화하지 않게 되므로 CMC 는 계면활성제의 중요한 특성이다. 또한, 계면활성제에 고분자 물질의 첨가는 이들 사이의 강한 정전기적 및 소수성 상호작용으로 인하여 계면활성제만의 CMC 보다 낮은 농도에서 마이셀을 형성하는데, 이와 같은 경우를 CMC 와 구분하기 위하여 CAC(critical aggregation concentration)라 부른다. 본 연구에서는 음이온 계면활성제인 SDS(Sodium dodecyl sulfate)에 PEO(polyethylene oxide)를 첨가함으로써 SDS 의 농도에 따른 PEO 의 행동을 점도, 표면장력, 전도도 측정 방법을 이용하여 살펴봄으로써 자화수의 특성을 알아보고자 한다.

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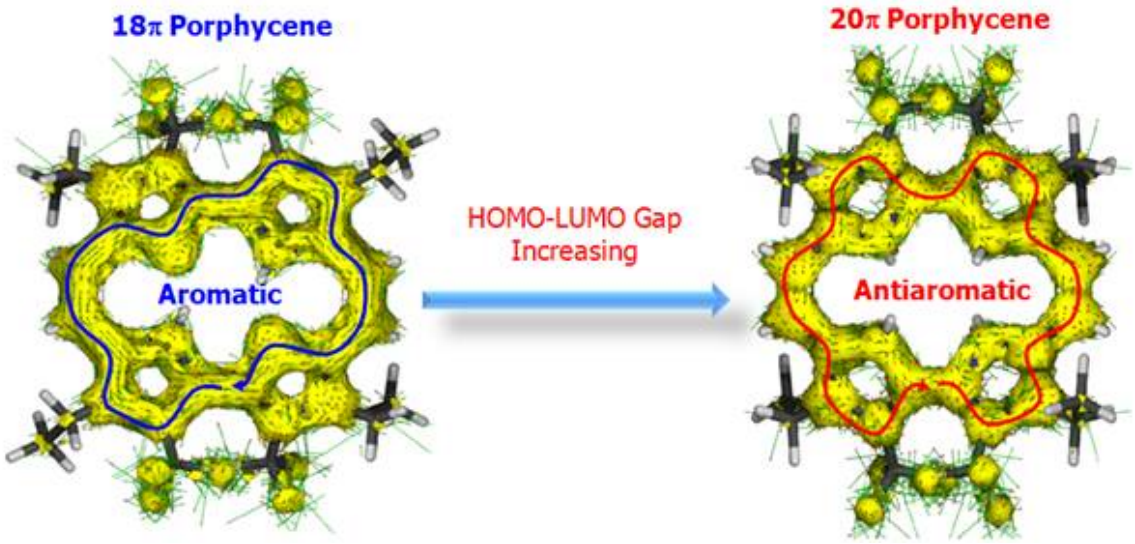
Comparative Photophysical Properties of Trifluoromethyl Substituted [18]/[20]π Porphycene Derivatives

김길석, 김동호

연세대 화학과

The photophysical properties of trifluoromethyl substituted [20]π porphycenes were investigated by theoretical calculations and spectroscopic measurements. Compared with other [4n]π porphyrinoids, [20]π porphycene molecule exhibits quite unique photophysical behaviors originating from a large HOMO-LUMO gap.



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Scanning ion-conductance microscopy to image neuronal cells

박애영, 이성훈

서울대 화학부

Currently, the exploration of living cells with a scanning probe microscope has been made in the respects of relationships between its 3D structure and function. Because the soft surface of biological macromolecules and cells is often easily damaged even during a tapping-mode scan, a mild surface-measuring scanning ion-conductance microscope (SICM) that utilizes a glass micropipette as the scanning probe has been developed. Since a SICM feedback maintains the working distance between the probe and the sample so that they do not make a direct physical contact at all, a SICM is suitable to image soft living cells without damaging them. Here we report the intact topography of neuronal cells using a SICM. This technique can be widely applied to the structural elucidation of soft materials such as living neuronal memorial cells.

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Theoritical Study of Amide-to-Ester Mutation on the designed Model Polypeptides

조예진, 함시현

숙명여대 화학과

The amide-to-ester mutation has been studied as a method for investigating the hydrogen bonding ability on the polypeptides. In this study, we compared the designed polypeptides for their structural and spectral properties when the mutation is occurred on the polypeptide backbones. All calculations were investigated by using density functional theory with B3LYP/6-31+G* level. Also, the effects of the mutation position on the model polypeptides will be discussed.

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Conformation Analysis of Sterically-hindered Amines for Quantitative Assessment of Their Steric Hindrance

전영호, 김자헌

숭실대 화학과

As an auxiliary agent in the absorption reaction between alkanolamine and CO_2, a sterically-hindered amine enhances both the overall reaction capacity and reaction rate because an easy hydrolysis of its carbamate can fix CO_2 as a bicarbonate ion in solution and regenerate sterically-hindered amine as well. This positive effect has been attributed to the large steric hindrance of the carbamate, which makes the compound weaker to a water attack compared with the carbamate of an unhindered alkanolamine. To quantify the magnitudes of the steric hindrance, B3LYP/6-31+G(d,p) relaxed scan calculations have been carried out to monitor variation of energies versus torsion angles for some selected amines. By analyzing these results, a correlation between the steric hindrance and their reactivity order has been suggested.

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Photophysical Properties of N-confused Hexaphyrins: Effects of Confusion of Pyrrole Rings and Molecular Shape on Electronic Structures

임종민, 김동호, *Hiroyuki Furuta

*연세대 화학과 *Kyushu university*

We have investigated the photophysical properties of N-confused hexaphyrins which are structurally modified by confusion of pyrrole rings compared with meso-hexakis (aryl) substituted hexaphyrins. On the basis of steady-state and time-resolved spectroscopic measurements, two-photon absorption (TPA) measurements and quantum mechanical (QM) calculations, we found out that electronic structures of hexapyrrolic macrocycles are perturbed by structural modifications. As a result of these electronic perturbations, N-confused hexaphyrins revealed broader absorption spectra and relatively shorter singlet excited-state lifetimes than their parent molecule. In the case of triply N-confused hexaphyrin, especially, the molecular symmetry is saliently modified; the rectangular shape of hexapyrrolic macrocycle is transformed into the triangular one with the introduction of triple N-confusions.

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Femtosecond Transient Absorption Study of Excited State Energy Transfer Dynamics for Organic/Inorganic Hybrid Complex

양일승, *강준희, **엄성수, **박주현, ***김성근

*서울대 화학부 *서울대 생물물리 및 화학생물학과 **중앙대 화학신소재공학부 ***서울대 화학부 & 서울대 생물물리 및 화학생물학과*

The organic/inorganic hybrid structures have recently attracted a great interest due to their many desirable materials properties. Charge transfer between metal oxide and dye is a key phenomenon to dye-sensitized solar cells and water splitting by photocatalysis for hydrogen fuel generation. Organic dyes tend to have a high cross section and a broad wavelength range for absorption that are essential in efficient harvesting of light. As charge acceptors, inorganic materials boast high efficiency and are readily available. We synthesized a porphyrin-metal oxide complex as a potentially promising model system for such organic/inorganic hybrid materials. We investigated the excited state energy transfer dynamics of this material by femtosecond transient absorption spectroscopy, with a particular attention paid to the comparison between the forward and backward transfer of electronic excitation.

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Structure and Phase Behavior of Binary Self-Assembled Monolayers Formed by Cyclohexanethiol and Adamantanethiol on Au(111)

김유영, 강훈구, 이남석, 노재근

한양대 화학과

Surface structures, adsorption conditions, and electrochemical behaviors of self-assembled monolayers (SAMs) formed by the adsorption of 1-adamantanethiol (AMT) and cyclohexanethiol (CHT) on Au(111) were characterized by means of scanning tunneling microscopy (STM), X- ray photoelectron spectroscopy (XPS), Termal desorption spectroscopy (TDS), contact angle (CA), and cyclic voltammetry (CV). CHT molecule has a flexible cyclic ring showing dynamic ring conformation, whereas AMT molecule has a rigid cage-like structure. To understand the competitive adsorption behavior of these molecules on Au(111), the binary SAMs were prepared as a function of relative molecular ratio of these molecules. Even though a lower mole fraction of AMT compared to CHT (40:60), SAMs were mainly formed by AMT. This result strongly implies the favorable adsorption of AMT molecules resulting from the enhanced van der Waals interactions between the rigid cage-like molecular backbones compared to CHT molecules.

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Solvent Effect on Formation of Alkanethiol Self-Assembled Monolayers on Au(111) at High Solution Temperature

이남석, 강훈구, 김유영, 노재근

한양대 화학과

Surface structure and electrochemical behavior of octanethiol (OT, $CH_3(CH_2)_7SH$) self-assembled monolayers (SAMs) on Au(111) after immersion Au(111) substrate in an ethanol, toluene, N,N,-dimethylformamide (DMF), and decane at 50 °C for 12 h were examined using scanning tunneling microscopy (STM) and cyclic voltammetry (CV) to understand the solvent effect on the formation of SAMs. The STM imaging and CV revealed that the property of solvent is very important in determining two-dimensional SAM structure. This result implies that the solvent is a crucial factor in growth of OT SAMs. Densely packed and well-ordered c(4 × 2) superlattice for OT SAMs was formed in ethanol, whereas, low-density striped phase was formed in toluene.

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Investigation of nanoenvironments in microheterogeneous media by single-molecule fluorescence microscopy

김성현, 정병서

인천대 화학과

The single-molecule fluorescence technique has been used to probe heterogeneity of molecular-scale nanoenvironments present in microheterogeneous media, in particular, hydrophilic polymer and sugar matrices that may be applied as matrices for encapsulation of biomolecules. Several different fluorescent dyes were employed as a sensitive spectroscopic probe of environmental properties. Fluorescence from single molecules were recorded as a function of time using the technique of fluorescence microscopy combined with a sensitive charge-coupled device(CCD) camera. Attempts have been made to reveal spatial or temporal variations in the local environment in the matrices by analyzing the sequential fluorescent images of single molecules, and the heterogeneous dynamics of the dyes are discussed.

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Preparation of stabilized TiO_2 nanoparticle suspension in aqueous solution

이노아, *윤민중, 송남웅

*한국표준과학연구원 미래융합기술부 나노바이오융합연구단 *충남대 화학과*

Colloidal nanoparticles (NPs) have high collision probability and their total surface area is larger than that of fixed NPs. And they act as more efficient catalyst in aqueous solution. To get highly concentrated and stabilized TiO_2 NPs dispersed in aqueous solution, we optimized dispersion process of agglomerated TiO_2 powder into aqueous suspension at various pH conditions. Dynamic light scattering method and the laser Doppler velocimetry were used for the measurement of hydrodynamic diameter and zetapotential of TiO_2 NPs in aqueous solutions depending on the preparation condition. UV/Vis absorption spectra were observed to compare the dispersity and concentration of TiO_2 supensions. It was observed that TiO_2 NPs were the most stable in the pH range of 8 to 10 with least re-agglomeration.

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Observation of phosphorylation site-specific dissociation of singly protonated phosphopeptides

신영식, *문정희, 김명수

*서울대 화학부 *한국생명공학연구원 단백체의학연구센터*

In ultraviolet photodissociation of phosphopeptide ions with a basic residue (arginine, lysine, or histidine) at the N-terminus, intense $a_n - 97$ peaks were observed. These ions were formed by cleavage at phosphorylated residues only. For multiply phosphorylated peptides, this site-specific cleavage occurred at every phosphorylated residue. H/D exchange studies showed that $a_n - 97$ was formed by H_3PO_4 loss from $a_n + 1$ radical cations. The site-specificity of phosphate loss observed here is in contrast with the nonspecific phosphate loss from b_n and y_n reported previously.

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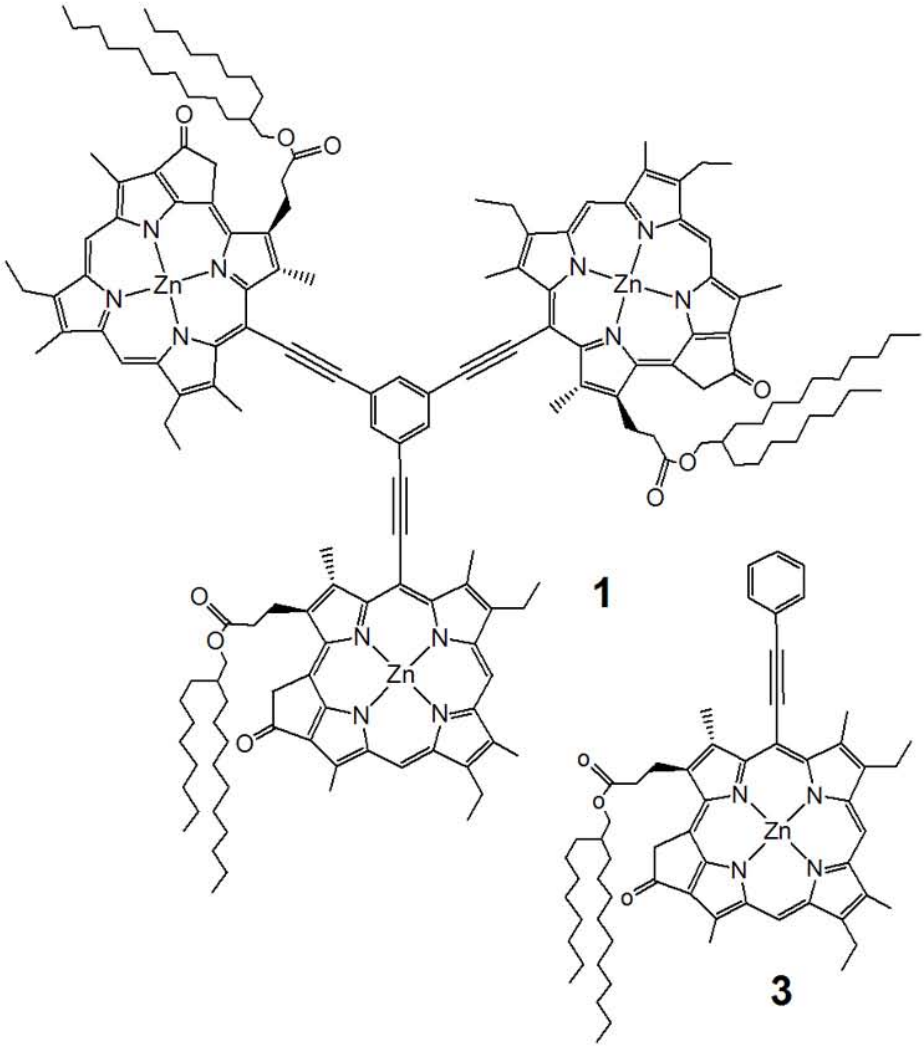
Fluorescence Dynamics of Chlorophyll Trefoils in the Solid State Studied by Single Molecule Fluorescence Spectroscopy

이지은, 양재성, *Victoria L. Gunderson, *Michael R. Wasielewski, 김동호

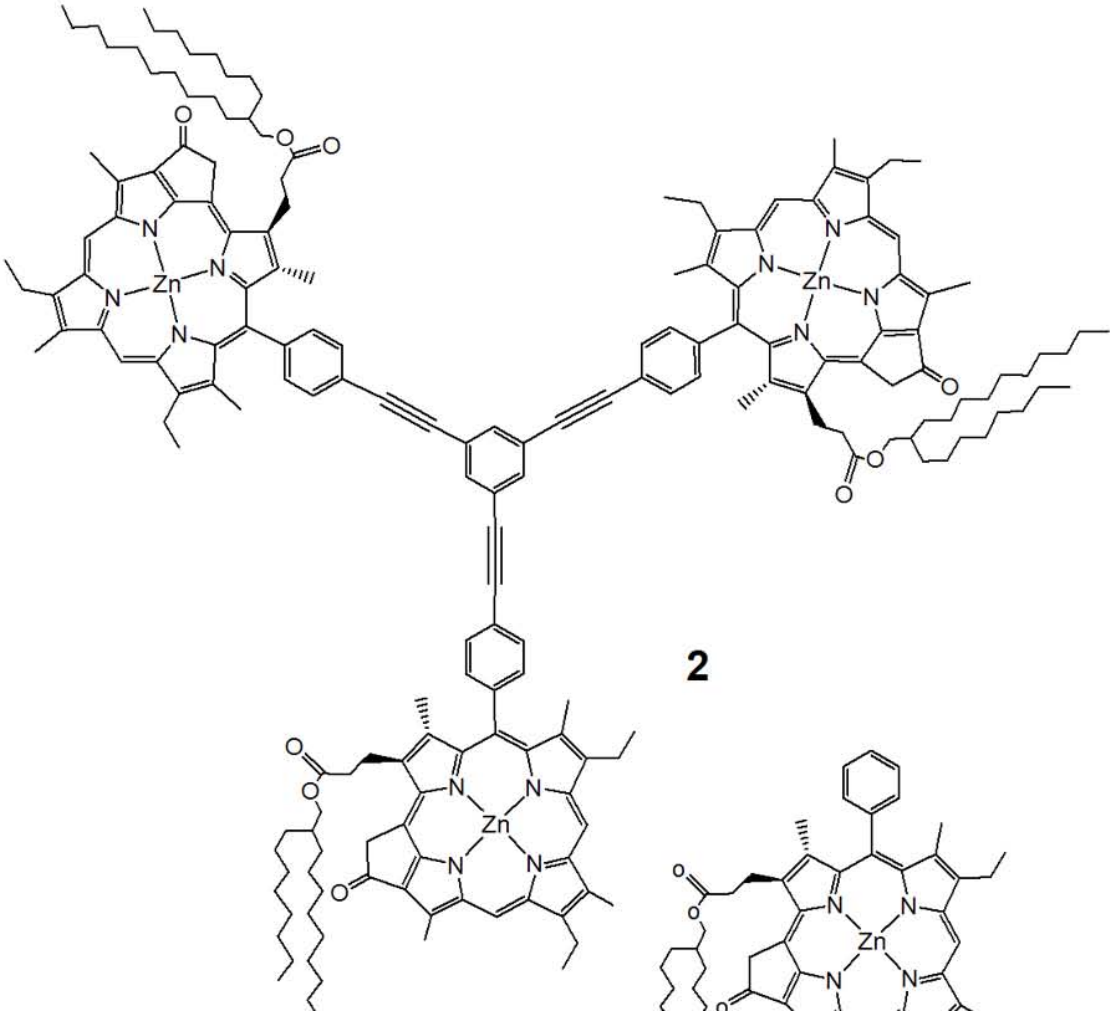
*연세대 화학과 *Northwestern University,USA (Department of Chemistry)*

We have comparatively investigated the single-molecule photophysical properties of two chlorophyll trefoils that feature distinctive electronic couplings induced by differences in linkage; one is an ethynyl linked chlorophyll trefoil (1) in which relatively short and rigid linkage between the chromophores promotes effective electronic coupling, and the other is a phenyl-ethynyl linked chlorophyll trefoil (2) in which the phenyl addition induces an orthogonal geometry impeding π-conjugation and provides a longer inter-chlorophyll distance reducing through-space interaction. By recording single-molecule fluorescence intensity trajectories and their corresponding lifetimes, we observed one-step photobleaching behaviors, less frequent on-off behaviors, a narrower fluorescence lifetime distribution, and higher photostability in 1 as compared with 2. These results indicate that the performance of molecular photosynthetic systems in the solid state is strongly associated with electronic couplings and thus, give insight into the construction of well-functioning artificial photosynthetic systems.



1

3



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Synthesis of Cerium Nanofibers by Electrospinning Technique

황아름, 조준모, 박주연, 강용철

부경대 화학과

Cerium oxide nanofibers were synthesized from poly vinyl alcohol (PVA) and cerium acetate (CA) hydrate solutions by using sol-gel processing and electrospinning technique. Electrospinning has been used as a simple and cost effective method for synthesizing nanfibers. The morphology and diameter of the cerium nanofibers were characterized by scanning electron microscopy (SEM), the crystal structure of the synthesized nanofibers was confirmed by XRD and the oxidation state, quantitative analysis, and the chemical environment of the obtained nanofibers were studied by XPS.

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Optimization of reflectron for kinetic and mechanistic studies with multiplexed multiple tandem (MS^n) time-of-flight mass spectrometry

배용진, 윤소희, *문정희, 김명수

*서울대 화학부 *한국생명공학연구원 단백체의학연구센터*

Photoexcitation of a precursor ion inside a cell floated at high voltage installed in a tandem time-of-flight (TOF) mass spectrometer provides triple tandem mass spectrometric information and allows kinetic and mechanistic studies. In this work, the factors affecting, or downgrading, the performance of the technique were identified. Ion-optical and computational analyses showed that an optimum instrument could be designed by utilizing a reflectron with linear-plus-quadratic potential inside. Theoretical predictions were confirmed by tests with instruments built with different ion-optical layout. With optimized instruments, masses of intermediate ions in the consecutive dissociation of a precursor ion could be determined with the maximum error of ±5 Da. We also observed excellent agreement in dynamical parameters (critical energy and entropy) for the dissociation of a model peptide ion determined by instruments with different ion-optical layout operated under optimum conditions. This suggests that these parameters can be determined reliably by the kinetic method developed previously when properly designed and operated tandem TOF instruments are used.

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Influence of basic residues on dissociation kinetics and dynamics of singly protonated peptides: time-resolved photodissociation study

윤소희

서울대 화학부

Product ion yields in post-source decay and time-resolved photodissociation at 193 and 266 nm were measured for some peptide ions with lysine ($[KF_6 + H]^+$, $[F_6K + H]^+$, and $[F_3KF_3 + H]^+$) formed by matrix-assisted laser desorption ionization. The critical energy (E_0) and entropy ($\Delta S^{\ddagger}$) were determined by RRKM fitting of the data. The results were similar to those found previously for peptide ions with histidine. To summarize, presence of a basic residue, histidine or lysine, inside a peptide ion retarded its dissociation by lowering $\Delta S^{\ddagger}$. Based on highly negative $\Delta S^{\ddagger}$, presence of intramolecular interaction involving a basic group in the transition structure was proposed.

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Molecular Dynamics simulation of HIV-1 Nucleocapsid protein with optimized force field parameters for zinc-binding interface

홍주연, 함시현

숙명여대 화학과

The human immunodeficiency virus-type 1 (HIV-1) nucleocapsid (NC) proteins contain two copies of an invariant array of CCHC that are crucial for RNA genome recognition, packaging, and infectivity and have been proposed to function as zinc-binding domains. Although the solution structures of the NC protein with Zinc binding have been determined by experimental studies, the physiological relevance of zinc coordination has not been revealed. Here, we present the structural characteristics of the NCp7 protein with Zn to investigate the coordination effect in the structural transitions upon inhibitory process by potential drugs by using molecular dynamics simulations with explicit water.

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Theoretical Studies on the Alkali Metal Cation Effects for the Reactions of Phenyl Aryl Chlorophosphates with Anilines in the Gas Phase and in Aqueous Solution

한인숙, 김창곤, 김찬경, *이본수, 이해황

*인하대 화학과 *인하대 총장실*

The Effects of Alkali-Metal Cation, X+ (=Li+, Na+, K+), for the substitution reactions of phenyl aryl chlorophosphates, C6H5OP(=O)(Cl)OC6H5, with anilines have been studied theoretically in the gas phase and in aqueous solution. All the reactions were found to proceed via a concerted mechanism with the nucleophile(aniline) and leaving group (Cl) occupying apical sites at the transition states (TS). On the contrary, for the reactions without X+, the TSs via a concerted process or any stable intermediates could not be located as stationary point species on the reaction coordinates. This indicates that the effects of X+ play a considerably important role. All the stationary point species have been fully optimized and characterized by frequency calculations at RHF level with 6-31+G(d) and at B3LYP level with 6-311+G(d) and 6-311+G(2d,p) basis sets.

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Effect of the oxygen gas ratio on the copper oxide films deposited on Si(100) surface

박주연, 조준모, 빈준형, 강용철

부경대 화학과

Copper oxide films were deposited on the p-type Si(100) using r.f. reactive magnetron sputtering as a function of different oxygen gas ratio in the sputter gas from 0 to 100%. The copper oxide films were investigated by atomic force microscopy (AFM), scanning electron microscopy (SEM), spectroscopic ellipsometry (SE), X-ray diffraction (XRD), and X-ray photoelectron spectroscopy (XPS). At the oxygen ratio of 0%, copper films are confirmed by XRD and XPS. After the oxygen sputter gas was introduced into the chamber, copper oxide films were deposited on the Si(100) substrate. The thickness of copper films was characterized by SEM and was found to be 650 nm. As the oxygen ratio increased, the thickness of the films was decreased that was checked by SE and SEM. The optical properties, refractive index of the Cu oxide thin films were also studied by SE. AFM images show that the surface of metallic copper films was rougher than that of Cu oxide films and the smoothness of the Cu oxide surface films were not affected by the oxygen ratio. The XRD data show the change of crystal structure from Cu through CuO and Cu_4O_3 mixing phase to CuO and Cu_2O. The Cu 2p and O 1s XP spectra show that the area ratio of CuO was larger than that of Cu_2O.

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Re-examination of MSEP method using semi-empirical method

Li Jun, 김창곤, *조수경, 이해황, 김찬경

*인하대 화학과 *국방과학연구소 4기술-2-1*

Recently, we have developed a novel QSPR method and applied this method to predict various physicochemical properties of organic and high energetic molecules. In this approach, molecular structures were optimized at B3LYP/6-31G(d) and electrostatic potentials were calculated on van der Waals molecular surface at the same level of theory (MSEP). Despite of its success, current MSEP scheme requires considerable computational time and thus has limited capability as a screening tool when applied to a large database. In this work, we first re-examined our approach to predict boiling points, fusion enthalpies, liquid densities, solid densities, sublimation enthalpies, and vaporization enthalpies of organic molecules using the semi-empirical methods such as AM1 and PM3.

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Ultraviolet lasing in ZnO nanowires at room-temperature

심형섭, 한노수, 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.

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Prediction of physicochemical properties of high energetic molecules using the semi-empirical method

김찬경, **Li Jun,** 김창곤, *조수경, 이해황

*인하대 화학과 *국방과학연구소 4기술-2-1*

Although numerous QSPR methods have developed to predict various physicochemical parameters of organic molecules, these methods could not be directly applied to high energetic molecules (HEMs). Therefore, we have developed a new QSPR scheme based on molecular surface electrostatic potential (MSEP). In this approach, molecular structures were optimized at B3LYP/6-31G(d) and electrostatic potentials were calculated on van der Waals molecular surface at the same level of theory. Despite of its success, current MSEP scheme has a limited capability to screen out promising HEM candidates from a large database. In this work, we re-examined our approach to predict various physicochemical properties of HEMs using the semi-empirical methods and compared with our previous results.

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Computational Study on the Conformational and Thermodynamic Features of D-amino acids Substitution in Model Dipeptides

이정은, 함시현

숙명여대 화학과

Molecular chirality is one of the key factors to control and to manipulate molecular functions in biological systems. Although L-amino acids are the predominant enantiomer in nature, D-amino acids have been found as neurotransmitters or building blocks for bacterial cell-membrane. Herein, we performed ab initio density functional theory (DFT) calculations at the B3LYP/6-31+G* level for 19 different model dipeptides containing a chiral center. We investigated conformational features of both L-forms and D-forms for model dipeptides and compared their thermodynamic stabilities depending on the side-chain substitutions with available experimental data.

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Determination of catalytic Activity of Ni contents on Ni/CeO_2 catalyst for CO_2 Reforming Reaction with Methane by Photoacoustic Measurements

강진규, 최중길, *이성한

*연세대 화학과 *연세대 화학 및 의화학과*

Photoacoustic spectroscopy was investigated for the determination of catalytic reaction of CO_2 reforming on different Ni weight percent of Ni/CeO_2. The catalysts were prepared by the adsorption method varing the Ni of 5, 7, 10, 12, and 15 wt% on CeO_2 powder. The reactions were performed in a closed-circulating reactor at total pressure of 40 Torr in the temperature range of 450 to 610 ℃. The acoustic signal generated in a photoacoustic cell was collected by using a condenser microphone and a lock-in amplifier, indicating the concentration changes of CO_2 gas during the catalytic reaction as a function of time. The apparent activation energies of each Ni/CeO_2 catalysts were obtained to optimize the amount of Ni on catalysts. The results of catalytic effect in the reaction were compared with the GC measurements in atmospheric pressure.

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Conformation of the 2-cyano-3-(thiophen-2-yl)acrylic acid used as an acceptor moiety for solar cells

김동희, 김세미, **Mannix Balanay**, 이미정, 이상희

군산대 화학과

A natural bond orbital analysis was performed on various dyes containing 2-cyano-3-(thiophen-2-yl)acrylic acid to provide a quantitative description of interactions that dictate the conformational features of the analogues. The increase in the electron delocalization between the thiophene and cyanoacrylic acid influences the stability for most of the analogues, except for NKX-2600, were its stability was mainly due to the presences of a weak hydrogen bond between the hydrogen of the methyl group of the amine located at the donor moiety and the nitrogen of the cyanoacrylic acid.

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Nonlinear optical properties of metallated tetraarylporphyrin analogues for solar cells

김동희, **Mannix Balanay**, 이상희

군산대 화학과

Nonlinear optical (NLO) donor-acceptor analogues containing porphyrin macrocycle as donor and cyanoacrylic acid as acceptor with varied π-bridging length were investigated to determine how these properties influence the observed light conversion efficiencies. The NLO properties were calculated using the Finite Field approach; they were influenced by the strengths of the donor and acceptor moieties and the length of the π-spacer group. The NLO response for all analogues was dominated by only one tensor component, indicating unidirectional charge transfer.

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Benzene의 진동수 모드에 대한 Ce+와 CeO+의 영향

이지현, *이기학, *서영선

*원광대 생명나노화학과 *원광대 화학과*

Benzene 을 포함하는 atomic cation ∏-상호작용은 구조화학과 생화학에서 꾸준히 관심받고있다.Benzene 은 생체분자 구조를 모방한 cation ∏ -상호작용 연구에서 원형이 되는 방향족 분자이다. 또한 최근에 별주위 대기 환경에서 Benzene 이 발견된다.성간가스(intersteller gas)에 있는 Benzene 과 금속 사이의 상호작용 중요성을 보여준다.Ce+와 Benzene 의 결합, CeO+와 Benzene 의 결합 특성과 Benzene 의 진동수 모드에 대한 Ce+와 CeO+의 영향을 보기위하여 혼성밀도 작용의 방법인 B3LYP(Guassian03)으로 계산 하였다.C,H,O 원자는 6-311+g* basis set 을 이용하였고 란타늄 원자는 stuttgart RSC segmented ECP 를 이용하였다.

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Theoretical study of Yb-benzen and Yb(C6H6)+n isomers

서영선, 이기학, *이지현

*원광대 화학과 *원광대 생명나노화학과*

Benzene 을 포함하는 atomic cation ∏-상호작용은 구조화학과 생화학에서 꾸준히 관심받고있다.Benzene 은 생체분자 구조를 모방한 cation ∏ -상호작용 연구에서 원형이 되는 방향족 분자이다. 또한 최근에 별주위 대기 환경에서 Benzene 이 발견된다.성간가스(intersteller gas)에 있는 Benzene 과 금속 사이의 상호작용 중요성을 보여준다.Yb+와 Benzene 의 결합, 결합 특성과 Benzene 의 진동수 모드에 대한 Yb+와 Yb benzen 의 영향을 보기위하여 혼성밀도 작용의 방법인 B3LYP(Guassian03)으로 계산하였다.C,H,O 원자는 6-311+g* basis set 을 이용하였고 란타늄 원자는 stuttgart RSC segmented ECP 를 이용하였다.

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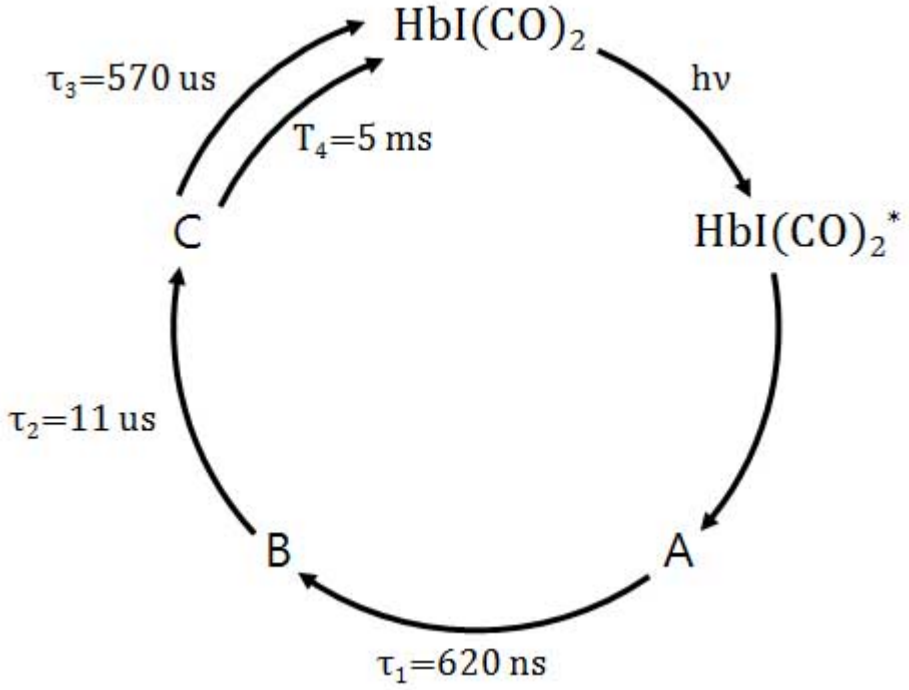
Direct observation of the allosteric effect by analyzing time-resolved X-ray solution scattering data

왕기영, *이효철

*KAIST 나노과학기술대학원 *KAIST 화학과*

We found that the decay of the third state (C) is biexponential. According to some previous literature, the fast one could be due to partially photolyzed T form of HbI (that is HbI(CO)) and the slow one could be due to fully photolyzed T form of HbI (that is HbI). Our TR-WAXS data could not have any definitive proof for that. In order to confirm it, we repeated the experiment with a lower laser power and found that the fraction for the fast-decay component increased. In summary, 1) our data confirms that both partially and fully photolyzed T form of HbI have the same molecular structures, and 2) our data provides a direct evidence that the partially photolyzed T form returns much faster than fully photolyzed T form. This is a direct proof of the allosteric effect.



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Visualizing E46Q PYP (Photoactive Yellow Protein) mutant photocycle by picoseconds time-resolved X-ray Laue Crystallography

정양욱, 손혜림, 이효철

KAIST 화학과

Visualizing the photocycle of PYP is important factor to understand its biological function as well as design photo-sensing materials. Time-resolved Laue crystallography has devoted to investigate photocycle and its signaling pathway for a long time. The previous success of WT (wild type)-PYP picoseconds time-resolved X-ray Laue crystallography encourages us to investigate a famous PYP mutant, E46Q, which has faster photocycle lifetime than that of WT-PYP due to deficiency of hydrogen bond. After photo-reaction of PYP is triggered by laser pulse (pump), the probe pulse (X-ray) can investigate the detailed structural changes. Finally, we determined kinetics at picoseconds regime in photocycle of E46Q PYP.

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Time-Resolved WAXS difference data fitting including the hydration layer – an explicit solvent molecular dynamics approach

GANESAN PRABHAKAR, 이재혁, 이효철

KAIST 화학과

At present there are no well established computer programs for Time-resolved Wide-Angle X-ray solution scattering (TR-WAXS) difference data fitting. All the existing methods deal mostly with the Small-Angle X-ray scattering (SAXS) data. TR-WAXS data is known to decode the secondary structural information of the proteins and is reported for its sensitivity in detecting the structural fluctuations of macromolecules in solution. Hence fitting of the TR-WAXS difference data to the structure might give us a realistic picture of structure dynamics of macromolecules in solution. Our goal is to develop module for fitting the TR-WAXS difference data using the Molecular Modeling Tool Kit (MMTK) based on all atom molecular dynamics approach. MMTK is a collection of open source program library written in the scripting language Python for molecular simulation applications. Since the hydration layer of the proteins have a significant contribution in the WAXS data, inclusion of the boundary water molecules in the fitting becomes essential. Thus the fitting of the TR-WAXS difference data must include the initial atomic coordinates of the protein molecules along with their respective hydration layer constituting of the explicit solvent molecules

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Adsorbate-Induced Changes in Surface Potential of Gold Nanoparticles Revealed by Raman Spectroscopy

신동하, *신권수, 김관

*서울대 화학부 *숭실대 화학과*

Noble metallic nanostructures exhibit a phenomenon known as surface-enhanced Raman scattering (SERS) in which the Raman scattering cross sections are dramatically enhanced for the molecules adsorbed thereon. When a molecule is adsorbed on these surfaces, its electronic structure changes dramatically, resulting in the shifting and splitting of spectral lines. Two further spectral changes can also be induced to occur by the application of an external electric field, one arising from the Stark effect and the other due to the bonding characteristics of the molecule onto the metal itself. The Stark effect and/or the changes in bonding characteristics should appear more distinctly in nanosystems than in bulk systems, because with smaller particles any applied electric field or excessive charge would remain confined. In this work, we demonstrate the characteristics and effectiveness of these changes by means of SERS. Specifically, the change in the surface potential of Au nanoparticles upon the adsorption of acetone and ammonia vapor is monitored by measuring the NC stretching frequency after fabricating 1,4-phenylenediisocyanide to sit in the gaps between planar Au and nanosized Au particles. The peak shift of the NC stretching mode turns out to be as much as 22 cm-1, corresponding to the variation of the surface potential of Au nanoparticles from +0.7 V to -0.6 V vs a saturated Ag/AgCl electrode. The peak shift observed must be attributed to the large surface-to-volume ratio of Au nanoparticles.

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REMPI Spectroscopy of Jet-Cooled 2-Aminophenol

김상수, *김민호, *손운용, 강혁, 박영동

*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) 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_2 group. Our calculation indicates that the trans isomer is much more stable than the cis isomer in the ground state, because the hydrogen boding structure in the latter involves rotation of NH_2 group with a high barrier. The REMPI spectrum shows the 0-0 band of 2AP at 33458 cm^{-1}, a strong 130 cm^{-1} progression, and a broad absorption feature at high excitation energy. The 130 cm^{-1} progression is assigned to the progression of 10a vibration (butterfly mode) based on the frequency calculation in the S1 state at the CC2 level. Calculation of Franck-Condon overlap integral successfully reproduced the experimental spectrum. The CC2 calculation also indicates that there is a $^1\pi\sigma^*$ state dissociative along the OH bond. In addition to the high density of Franck-Condon active vibrational states at high excitation energy, the dissociation of H atom also contributes to the lifetime broadening of the REMPI spectrum.

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Solvent-Assisted Conformational Isomerization of 3-Aminophenol

김민호, *김상수, 손운용, *강혁, *박영동

*아주대 에너지시스템학부 *아주대 화학과*

When 3-amionphenol (3AP) makes a cluster with a proton-accepting solvent, a hydrogen bond is formed between the solvent and the H of the hydroxyl group in 3AP. In previous experiments, while the 0-0 transition of *cis*-3AP was found in the REMPI spectrum, the 0-0 transition of *cis*-3AP-H2O or *cis*-3AP-NH3 was not observed. It is assumed that the *cis* conformer of the cluster isomerizes to the more stable trans conformer in the ground state. The binding energy of the cluster is available as the excess energy to overcome the isomerization barrier. We attached several molecules which can make hydrogen bonds to 3AP and observed the conformational isomerization as a function of binding energy calculated at MP2 level.

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Computational Study of 3-Aminophenol•$(CO_2)_1$ Cluster

손운용, *강혁

*아주대 에너지시스템학부 *아주대 화학과*

The structure of -Aminophenol•$(CO_2)_1$ cluster was computationally studied in the ground and the lowest singlet excited electronic states. The ground state structure and binding energy of the cluster was investigated using the second-order Möller–Plesset perturbation theory (MP2) at the complete basis set (CBS) limit. The excited state geometry of the cluster was obtained at the second-order approximate coupled cluster (CC2) level with cc-pVDZ basis set, and the S0-S1 absorption spectrum was simulated by calculating Franck-Condon overlap integral. Only one stable ground state geometry with a very high binding energy of 4.3 kcal/mol was found for the cluster, due to the strong π- π interaction between the aromatic ring and CO_2. The excited state geometry shows a very big shift in the position of CO_2 compared to the ground state geometry, which results in low intensity and broad envelope in the Franck-Condon simulation. The preliminary experimental S0-S1 spectrum in our group agrees with the FC calculation.

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Aluminum Oxide Submicro-Rings synthesized by electospinning.

조준모, 황아름, 박주연, 강용철

부경대 화학과

We have synthesized uncommon form of nano-material which is ring shape by electrospinning technique. To our knowledge, there were no reports about the preparation and investigation of alumina submicro-rings by electrospinning technique. The size of rings was observed by scanning electron microscopy (SEM) and found to be in the range from nano- to submicro- meters. The aluminum oxide submicro-rings (sm-rings) produced after electospinning and calcination at different temperatures, such as 573K, 873K were characterized by X-ray diffraction (XRD) and X-ray photoelectron spectroscopy (XPS). XRD data show that only aluminum phase was observed and the intensity of the peaks was dependent on the calcinations temperature. The XP Spectra reveals that the aluminum oxide ratio was increased with increasing calcination temperature.

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Investigation of MoO_x Thin Films for CIGS Applications

빈준형, 박주연, 조준모, 강용철

부경대 화학과

Molybdenum oxide thin films were deposited on p-type Si(100) wafer by radio frequency magnetron sputtering method. The physical and chemical properties of these films were studied with X-ray diffraction (XRD) and X-ray photoelectron spectroscopy (XPS) techniques. At the oxygen ratio of 0%, molybdenum thin film which has cubic Mo (110) peaks was observed by XRD. After the oxygen ratio was 20%, the molybdenum oxide thin films were amorphous phase. The thickness of molybdenum oxide thin films was measured by spectroscopic ellipsometer (SE) and scanning electron spectroscopy (SEM) and the thickness was found to be 1 μm. When the pressure of oxygen gas in the sputter gas increased, the film thickness was decreased upto ~55 nm. The ratio of metallic Mo decreased but the contents of Mo6+ species increased as the oxygen gas ratio increased.

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Growth of carbon nanotubes from Ni nanoparticles and C_2H_2 by thermal chemical vapor deposition

정승환, 이상국

부산대 화학과

Multiwalled carbon nanotubes(MWCNTs) were grown by the thermal chemical vapor deposition. The Ni was used as a catalyst and the mixture of H_2/C_2H_2(gas phase) was a carbon source. We conduct an experiment that the temperature was 50℃ gap from 650℃ to 900℃ and the reaction time was 5,15,30 minutes. The effect of temperature and reaction times on surface morphology has been investigated. We used scanning electron microscopy(SEM), high-resolution transmission electron microscopy(TEM), energy dispersive spectroscopy(EDS) and atomic force microscopy(AFM) to observed continuous increase in density and decrease in size of carbon walls with increasing temperature.

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Ultraviolet photodissociation action spectroscopy of protonated tyrosine cations at a cryogenic temperature using quardrupole ion trap reflectron time-of-flight mass spectrometry

최대호, 김남준

충북대 화학과

The ultraviolet (UV) photodissociation action spectrum of protonated tyrosine ion was obtained in the gas phase using quadrupole ion trap reflectron time-of-flight mass spectrometry. The protonated tyrosine ions produced by electrospray ionization were stored in the quadrupole ion trap (QIT) cooled down to ~10K by a closed cycle helium refrigerator. In order to obtain the photodissociation action spectrum, the UV beam was irradiated onto the ions in the QIT and the ion signals of the fragment ions were monitored as a function of the UV wavelength. The action spectrum exhibited well-resolved vibronic peaks. By simulating the band contour of the origin band of the S_0-S_1 transition, the temperature of the protonated tyrosine ions in the cold QIT was determined to be around 35K.

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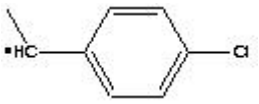
Identification of p-Chloro-α-methylbenzyl Radical in Corona Excitation

윤영욱, 이상국

부산대 화학과

Identification of new transient molecular radical is one of the most difficult job in experimental spectroscopic work because they show extremely short life time, high reactivity and very low concentration in the gas medium. We have obtained the vibronic emission spectra from the corona discharge of p-chloroethylbenzene and p-chlorotoluene seeded in a large amount of inert carrier gas by employing a pinhole-type glass nozzle in a corona excited supersonic expansion. By comparing both spectra observed from each precursor, we have identified the existence of p-chloro-α-methylbenzyl radical in the jet which could be produced by losing hydrogen atom from methyl group at α-position. The mechanism of new aromatic molecular radical from precursor will de described in the presentation.



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Isomerization and dissociation of the phenylarsane molecular ion: a DFT study

김선영, 최중철

동국대 화학과

We have explored the potential energy surface (PES) for the isomerization and dissociation of phenylarsane molecular ion. The EI mass spectrum of phenylarsane shows strong peaks corresponding to loss of H_2 and AsH with intermediate ones corresponding to loss of H and As. Quantum chemical calculations at the B3LYP/6-311+G(3df,2p)//B3LYP/6-31G(d) level showed that the loss of H_2 was the most favored dissociation channel. According to the PES, six-membered ring intermediates were important in all the major dissociation channels and seven-membered ring intermediates also played a role in the loss of H. Based on the PES, the dissociation kinetics will be discussed to explain previous experimental results.

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The growth of CNT three-dimensional networks on various substrates.

여해구, 서정은, *이태재, 이해원

*한양대 화학과 *한양대 나노과학기술연구소*

CNT three-dimensional (3D) networks which grown on Si substrate is useful for electronics, optics, sensor and material science. But some properties of Si substrate has limitation in many application fields. So the growth of CNT 3D networks on various substrates is needed to overcome this limitation. In this study, CNT 3D networks were grown by low pressure thermal chemical vapor deposition (CVD) on various substrate such as Si, SiO_2, quartz and sapphire. Fe-Mo were used as the cocatalyst and deposited on substrate by a dipping method. In CVD process, C_2H_2 gas was used as a carbon source to grow CNT 3D networks after NH_3pretreatment at 800 ℃. The CNT 3D networks were characterized by scanning electron microscopy (SEM), and Raman spectroscopy.

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Energy transfer dynamics of OLED devices

서주희, 한노수, 심형섭, 박승민, 송재규

경희대 화학과

Phosphorescence in organic materials is distinguished from fluorescence by its origin in forbidden transitions that violate spin conservation. The excited states responsible for phosphorescence and fluorescence are named after their spin multiplicity as triplet and singlet states, respectively. Since the electrical excitation generates three triplet states for every singlet state, the properties of triplet states are of interest for their application to organic optoelectronic devices. For development of phosphorescent organic light emitting diode (PHOLED), we investigated the energy states and energy transfer dynamics between composites in PHOLEDs. Specially, the energy transfer dynamics between m-MTDATA and Ir(ppy)3 was studied in detail at low temperature (10 K) and room temperature (300 K), because m-MTDATA and Ir(ppy)3 are the widely-employed host and dopant molecules. The energy transfer from m-MTDATA to Ir(ppy)3 was found to be followed by the energy transfer from Ir(ppy)3 to m-MTDATA, which was observed by time-resolved photoluminescence spectroscopy.

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Details of the Chain Transfer Reaction during Radical Polymerization of Polyvinylpyrrolidone by Two-Dimensional IR-NMR Heterospectral Correlation Spectroscopy

박근우, 홍원진, 유수련, 정영미

강원대 화학과

In this presentation, the mechanism of chain transfer reaction during radical polymerization of vinylpyrrolidinone was studied. AgNO3 used as a chain transfer agent was reduced to form nanoparticles by the in-situ electron transfer reaction. To investigate the formation of C=C double bond during radical polymerization, we have applied two-dimensional (2D) correlation spectroscopy to the time-dependent FTIR and 1H NMR spectra of chain transfer reaction during radical polymerization of vinylpyrrolidinone.Results of 2D IR-NMR hetero-spectral correlation analysis shows the formation of C=C double bond during radical polymerization, which reveals clearly the mechanism of chain transfer reaction.AcknowledgementsThis work was supported by National Research Foundation of Korea Grant Funded by Korea Government (No. 2009-0087013) and the BK 21 program from the Ministry of Education, Science and Technology of Korea.

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Study on the pH-dependent bovine α-lactalbumin by using Raman optical activity and IR spectroscopies

유수련, [*]B. Czarnik-Matusewicz, [**]Rina K. Dukor, 정영미

강원대 화학과 [*]Faculty of Chemistry, University of Wroclaw [**]BioTools Inc., Jupiter, FL 33458

Raman optical activity (ROA) measures vibrational optical activity by means of a small difference in the intensity of Raman scattering from chiral molecules in right and left circularly polarized incident laser light. Proteins in aqueous solution are now accessible to ROA measurements, which provide an incisive new probe of secondary and tertiary structure. 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 IR and ROA spectra of the pH-dependent bovine α-lactalbumin to investigate the molten globule state. The details of molten globule state of bovine α-lactalbumin will be discussed. It is a key issue to understand bases of the secondary structure changes that are responsible for various conformational diseases. AcknowledgementsThis work was supported by National Research Foundation of Korea Grant Funded by Korea Government (No. 2009-0065428 and No. 2009-0087013) and the BK 21 program from the Ministry of Education, Science and Technology of Korea.

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Controlled Chemical Formation of Atomic Defects in Graphene and their Optical Characterization

고택영, *안광현, *류순민

*경희대 응용화학부 *경희대 응용화학과*

Graphene, a single layer of graphite, has recently induced a lot of research efforts towards understanding its unique physical properties. Chemical understanding and manipulation of this new material, required to realize its potential, has been lacked so far. To develop a simple and reliable method to introduce robust atomic defects in the basal plane of graphene, reaction of oxygen radical with graphene has been explored by Raman spectroscopy and scanning probe microscopy. Oxygen atoms were generated in situ by UV photolysis of oxygen molecules. The reaction leads to a strong Raman D band in graphene, which indicates the formation of presumably atomic point defects. Further studies are being carried out to pinpoint chemical identities of the new surface oxides and quantify the atomic defects. This study will be of great significance to those who are interested in the chemical manipulation of graphene.

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Characterization of Cathode Surface of Li-Ion Battery under High Voltage Condition by Two-Dimensional Correlation Spectroscopy

김남훈, 박연주, *최현철, 정영미

*강원대 화학과 *전남대 화학과*

Li-ion batteries have been widely used to commercial energy device. Therefore the improvement of Li-ion batteries safety is one of the key issues for the establishment of portable electronic instruments and electric vehicles. Li-ion batteries safety is intensely relative to the instability of charged cathode or anode, in presence of liquid electrolyte. Especially overcharged Li-ion battery has been studied most extensively, but the overcharge mechanism is still not clear. In this presentation, we have applied 2D correlation spectroscopy to the Raman and XPS spectra of Li-ion battery to investigate the overcharge behavior on the cathode surface. The overcharge mechanism of cathode of Li-ion battery will be discussed in more detail.AcknowledgementThis work was supported by Agency for Defense Development, Korea, National Research Foundation of Korea Grant Funded by Korea Government (No. 2009-0087013), and the BK 21 program from the Ministry of Education, Science and Technology of Korea.

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Application of SERS immunoassay for detection of PSA

서형균, 홍원진, 정영미

강원대 화학과

Surface-enhanced Raman scattering (SERS) technique provides 10^6–10^{14}-fold enhancement in Raman signal intensity. SERS has been used for the analysis of molecular information through sharp and easily distinguishable vibrational bands and also for bioanalyte detection. The use of normal Raman scattering as a readout method for immunoassays is limilted by low intensity and lack of sensitivity. In this study, colloidal gold nanoparticles were prepared by reducing gold chloride hydrate with trisodium salt dehydrate. These particles have excellent optical properties for a sensitive detection of Prostate-Specific Antigen (PSA) as a biomarker. Highly sensitive immuno-analysis of these complexes was performed using SERS. In this presentation, details of immunoassay techniques based on the SERS will be discussed.AcknowledgementsThis work was supported by National Research Foundation of Korea Grant Funded by Korea Government (No. 2009-0083707) and the BK 21 program from the Ministry of Education, Science and Technology of Korea.

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Characterization of Biodegradable Poly(3-hydroxybutyrate-co-3-hydrohexanoate) and Poly(Ethylene Glycol) Blends by Two-Dimensional Correlation Spectroscopy

김민경, 유수련, *Isao Noda, 정영미

*강원대 화학과 *Procter & Gamble Company*

Poly(3-hydroxybutyrate) (PHB) has been studied extensively as an environment-friendly polymers. PHB-based copolymers, such as poly(3-hydroxybutyrate-co-3-hydrohexanoate) (P(HB-co-HHX)), has recently been introduced. Poly(ethylene glycol) (PEG) has advantages of biocompatibility, biodegradability, and hydrophilicity. P(HB-co-HHx)/PEG blends with a PEG content of 2, 10, and 20 wt% were prepared from chloroform solution. It is of importance to investigate the thermal behavior of biodegradable materials, because the mechanical properties and chemical stability of a crystalline polymer strongly depend on the crystal structure and morphology. In this study, to investigate thermal behavior of P(HB-co-HHx)/PEG blend, 2D correlation spectroscopy was applied to the temperature-dependent IR spectra of thin films of P(HB-co-HHx)/PEG blend.*AcknowledgementsThis work was supported by National Research Foundation of Korea Grant Funded by Korea Government (No. 2009-0065428) and the BK 21 program from the Ministry of Education, Science and Technology of Korea.*

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Enhanced Chemical Reactivity of Rippled Graphene Studied by Raman Spectroscopy

안광현, 송지은, 류순민

경희대 응용화학과

Graphene has drawn a great interest for its potential application in future electronics. Since graphene supported on a solid substrate is generally observed to be rippled on the nanometer scale, the influence of the structural deformation on its various properties is an important issue to be resolved. In this study, chemical activity of rippled graphene has been investigated by Raman spectroscopy. Nanometer scale corrugation was induced by thermal treatment exploiting differential thermal expansion between graphene and Si substrates. Oxygen atoms generated by UV photolysis of oxygen molecules were used as reactants, which attack the basal plane of graphene to form structural defects. The degree of the reaction was quantified by the disorder-related Raman D band. The observed enhanced reactivity of rippled graphene suggests that material properties of graphene can be manipulated by controlling morphology of graphene.

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Fabrication of Vertically Aligned Petal-like Carbon Nanowalls(PCNWs) Using Microwave Plasma Enhanced Vapor Deposition(MPECVD) on Si Wafer without Catalyst Layer

허창순, 이상국

부산대 화학과

We investigated the growth process of petal-like carbon nanowalls (PCNWs) on a Si substrate by microwave plasma-enhanced chemical vapor deposition (MPECVD). It is revealed that the PCNWs are grown at the fine-textured structure on the Si and the growth process does not require the catalyst. The PCNW initially has a semicircular shape. The height, thickness, and mesh size increase with growth time. In the case using C_2H_2/H_2 system, aligned petal-like carbon nanowalls (PCNWs) were grown vertically on the substrate. It is found that the height of PCNWs as a function of time obeys the square root law. Scanning electron miscroscopy (SEM), energy-dispersive spectroscopy (EDS), and atomic force microscopy (AFM) were used to analyze the CNT morphology and composition.

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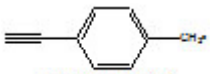
Observation of Benzyl-type Radical in a Corona Excitation

이승운, 이상국

부산대 화학과

Benzyl radical, the prototype free radical, has been recognized for a long time to be reaction intermediate in aromatic chain reaction and the subject of numerous spectroscopic studies. The corona excited supersonic expansion, well-developed in this laboratory has been employed to produce jet-cooled benzyl-type radicals from precursors seeded in a large amount of inert carrier gas. The ethynylbenzyl radical was generated from the precursor ethynyltoluene with a large amount inert gas helium using a pinhole-type glass nozzle in a CESE. The visible vibronic emission spectra were recorded with a long-path monochromator for o-, m-, and p-isomers. The spectra were also compared with the cyanobenzyl radicals which have a total of 7 delocalized π electrons in the molecular plane and analyzed to give an accurate electronic and vibrational mode frequencies.



p-ethynylbenzyl radical

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Doubly β-functionalized meso-meso Directly Linked Porphyrin Dimer Sensitizers for Photovoltaics

박선우, 김동호

연세대 화학과

A novel meso-meso directly linked porphyrin dimers tethered at β-pyrrolic position of porphyrin ring with 2-propenoic acid or 2,4-pentadienoic acid were prepared for sensitization of nanocrystalline titanium dioxide solar cells. Most importantly, the absorption spectra of dimeric porphyrins notably were extended into mid-visible region in solar spectrum while the LUMO levels are sufficiently high to inject electrons to the conduction band of TiO_2. Among these dimers, PEG-2b-bd-Zn2 dimer bearing polyethyleneglycol end group at one meso position showed the highest incident photon-to-photocurrent generation with 47% efficiency at Soret region as well as the conversion efficiency of 4.2% under standard AM1.5 solar condition. To elucidate electronic structures and excited state properties, UV-vis absorption and emission, and density functional theory calculation were performed. To our best knowledge, the obtained conversion efficiency of 4.2 % from PEG-2b-bd-Zn2-sensitized DSSC is the highest photovoltaic performance among DSSCs based on oligomeric porphyrins. Thus, this work suggests that the wide spectral response of directly linked porphyrin dimers due to the excitonic coupling is an intriguing aspect of directly linked pophyrin dimers to be utilized for DSSCs and gives an insight into the design of more efficient light harvesting molecules.

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Self-Assemble Monolayers of Halo-Substituted Aromatic Thiols on Au(111)

강훈구, 김유영, 이남석, 조철호, 이성근, 노재근

한양대 화학과

Self-assembled monolayers (SAMs) prepared by aromatic thiols on gold surfaces have much larger potential for electronic device applications due to their electronic properties. In this study, the formation and structures of SAMs prepared by pentafluorobenzenethiol (PFBT), 4-fluorobenzenethiol (4-FBT), pentachlorobenzenethiol (PCBT), and 4-chlorobenzenethiol (4-CBT) on Au(111) were examined using scanning tunneling microscopy to explore the impact of a slight variation of molecule size and substituent electronegativity. It was found that the immersion temperature, time, and concentration of the solution play a major roll in determining the surface structure of two-dimensional (2D) ordered SAMs. It was revealed that all four thiol-molecules form uniform SAMs on Au(111) at 75 °C compared to lower solution temperature. We clearly demonstrated that PFBT molecules on Au(111) at 75 °C can form 2D ordered SAMs, which can be described as a $(2 \times 5\sqrt{13})R30°$ structure, whereas PCBT SAMs have a $(\sqrt{13} \times 2\sqrt{5})R46°$ packing structure.

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One-photon Ionization Spectroscopy of Bromocyclohexane: the Origin and Quantitative role of Conformational Anomeric effect

한송희, *유현식, 김상규

*KAIST 화학과 *KAIST 화학과*

The VUV-MATI spectroscopy of bromocyclohexane was performed to give precise and accurate ionization potentials for chair- equatorial(9.8302 ± 0.0025 eV) and axial(9.8404 ± 0.0025 eV) conformers of bromocyclohexane molecule. The equatorial is more stable than axial in both neutral and cationic ground states while it has undergone severe structural change compared to the other conformer. The origin of this observation is from larger anomeric effect between n*(Br) and $\sigma_{C\ Br*}$ orbitals of equatorial in the cationic ground state. Tthe quantitative role of anti bonding orbital, $\sigma_{C\ Br*}$ is revealed by using the NBO calculation. The C-Br torsional motion is strongly observed in equatorial and ring puckering is an activated mode in axial. The SOMO of axial is almost same with HOMO, however, those of equatorial are different each other, implying the drastic structural change of equatorial only, which is due to the trend of increasing the anomeric effect and decreasing the steric effect for more stabilization, supporting the above explanation for ionization driven conformer specificity of equatorial and axial bromocyclohexane molecules.

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The study of intramolecular charge-transfer dynamics in Alkynylpyrene derivatives

성주영, *김종승, 김동호

*연세대 화학과 *고려대 화학과*

Intramolecular charge transfer dynamics in donor-acceptor system have attracted a great interest. Alkynylpyrene derivatives consisting of Pyrene, as an acceptor moiety, N, N-Dimethyl aniline, as a peripheral donor moiety, and ethynyl group as a bridge, was prepared as a D-π-A system. We have measured steady state absorption, fluorescence emission, and Time-resolved fluorescence experiment to investigate to ICT character. By adding the peripheral donor moiety, altering substituent position and using various solvents, we could identify the ICT character.

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SERS Study of Photoisomerization of Azobenzene Derivative in Gold Nanoparticle Aggregates

윤준희, 윤상운

단국대 화학과

We report a photoisomerization reaction of azobenzene derivatives (Az) in gold nanoparticle (AuNP) aggregates and the subsequent structural changes of the AuNP aggregates and the molecules. Stable AuNP aggregates are induced by the addition of synthesized azobenzene derivatives with a spacer and a sulfide group. Upon irradiation at 365 nm, Az transforms from *trans* to *cis*, confirmed by the appearance of the characteristic cis band at 586 cm^{-1} in SERS spectra. In addition, UV-Vis absorption dramatically increases in the long wavelength region, indicating that the photoisomerization of Az brings the AuNPs closer in the aggregates. Furthermore, red shifts of N=N stretch modes in the SERS spectra upon irradiation suggest that the isomerization to a *cis* form leads to the binding of the N=N bond to the neighboring AuNPs, weakening the bond. Much faster thermal back isomerization of *cis* in aggregates than in solution is consistent with the structural changes of the AuNP aggregates and the Az.

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Raman Spectroscopy Study of Grpahene on Atomically Flat Mica

심지혜, 송지은, 류순민

경희대 응용화학과

Graphene, one single atomic layer of graphite, has attracted significant interest since its recent discovery. Its unique electronic structure and properties render graphene a fascinating material for various applications such as chemical sensors, transparent electrodes and field-effect transistors (FETs). Ripples of graphene on the nm scale are thought to affect its various properties. Here we report a Raman spectroscopy study of graphene supported on atomically flat substrates. Ultraflat graphene was prepared by micro-exfoliation of graphite followed by deposition on cleaved mica surfaces. Atomic force microscopy (AFM) was exploited to reveal detailed morphology of high-quality graphene on mica. The effect of environmental charge doping in graphene was investigated by Raman spectroscopy. This study will increase our knowledge on the properties of graphene and eventually contribute to realization of useful applications based on graphene.

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Comparative DFT study for molecular Geometries of Methyl Peophorbide-a: Testing of M06-2X Functional and 2 Others Functional

조은애, 허도성, *최상준

*인제대 화학과 *인제대 의생명화학과*

Recent interest in application of density functional theory prompted us to test several functionals in molecular geometries of methyl peophorbide-a(MPa). In the present study, we report such test for popular 3 DFT functionals(M06-2X class levels, B3LYP class levels, and LSDA class levels) We draw the following conclusion based on the standard deviation of difference from experimental value and the mean of the difference in geometries. M06-2X class level s have the smallest standard deviation of difference among the used DFT calculation in bond length, whereas the standard deviation of bond angle in LSDA/6-311+G(d,p) is the smallest the standard deviation among the DFT. However, the mean value of LSDA calculation is larger than that of M06-2X in absolute value. Then M06-2X/6-311+G(d,p) give best performance for MPa. MPa is an important material as Photodynamic Therapy (PDT) and starting materials of PDT. MPa is more attractive photosensitizer because of its absorbance band at 668 nm. The UV-Visible band calculated with TD DFT class levels. TD M06-2X/6-311+G(d,p) give also best performance for MPa in solution.

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Femtosecond Nano tip Electron Microscopy Using Shear force Control

정다희, *연기영, *김상규

*KAIST 화학과 *KAIST 화학과*

Femtosecond-resolved Nano tip electron Microscope provides nanometer spatial and femtosecond temporal resolution.In this study, we manufacture tungsten nano tip using electrochemical etching system and it used for generating the free electron with femtosecond laser pulses and taking surfaces images in shear force microscopy. We can control the distance between the nano tip and the sample using the shear force microscope system. By using the shear force microscopy we acquired Nickel mesh and line patterned SIN. Also by accomplishing electron pulse characterization, we confirmed that the quantities of electron pulse depends on the injected laser intensity and the bias voltage supplied to the nano tip. Our final goal is time-resloved surface imaging using pump-probe method. By using this technique we will analysis reaction occur on surface in real time and space.

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Pt- and CdS-Nanodiamond Hybrid Nanostructures with High Photocatalytic Activity Under Visible Light Irradiation

장동명, 김윤희, 명윤, 조용재, 김한성, 박정희

고려대 소재화학과

Platinum (Pt) and cadmium sulfide (CdS) nanocrystals (NCs) were grown in situ on acid-purified detonation nanodiamonds (NDs, diameter = 5 nm) by the solvothermal method. The Pt-ND and Pt-CdS hybrid nanostructures exhibit the higher photocatalytic activity (about 1.5 times) than the matching TiO_2 and CNT hybrid nanostructures, toward the visible-light-driven degradation of methylene blue. X-ray photoelectron, Raman, and IR spectroscopy suggest the stronger binding interaction of NDs with the NCs, involving the carboxylate or ester type ionic forms, which induces a more efficient interfacial electron transfer process that is responsible for the enhanced photocatalytic activity. The defective surface structure of NDs would further increase the oxidative degradation rate of Pt-ND hybrid nanostructures.

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Molecular Shape-dependent Photophysical Properties of *meso*-β Doubly Linked Zn(II) Porphyrin Arrays

허지행, 임종민, *Atsuhiro Osuka, 김동호

*연세대 화학과 *Kyoto University*

The covalently linked Zn(II) porphyrin arrays in which the porphyrin macrocycles are doubly linked at *meso*-β, *meso*-β positions are investigated by steady-state and time-resolved spectroscopy along with quantum mechanical calculations in order to reveal their shape-dependent photophysical properties. Similar to other covalently porphyrin arrays, *meso*-β doubly linked Zn(II) porphyrin arrays exhibit a systematical spectral changes, but the syn-type trimers shows a unique photophysical properties. Syn-type trimer presents almost the same values of the S_1-state lifetime and the TPA values with the dimer, as revealed by time-resolved spectroscopic measurements, supporting that the syn-type trimer behaves as the dimer. The TD-DFT calculation results clearly proved that the syn-type trimer has a different electronic structure compare with the corresponding anti-type trimer, we confirm that the syn-type trimer is composed of the two independent dimer units.We also synthesized a new type of porphyrin arrays in which benzene ring is fused at the *meso*-β position of the porphyrin to evaluate the ring fusion effect influences to the non-fused doubly linked porphyrin arrays. It was found that the benzene-fused arrays exhibit the enhanced TPA values and shortened S_1-state lifetime because of the elongated π-conjugation and perturbation of the electronic structures. Our research provides further insight into the molecular shape-dependent electronic properties of not only the *meso*-β doubly linked Zn(II) porphyrin arrays but also of covalently linked porphyrin array system.

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Localized Surface Plasmon Mapping of Ag-Au-Ag Heterometallic Nanorods

김덕수, 김지환, *송현준, *서대하

*고려대 화학과 *KAIST 화학과*

We use scattering-type apertureless near-field scanning optical microscopy (s-ANSOM) to study localized surface plasmons of Ag-Au-Ag heterometallic nanorods. An atomic force microscopy (AFM) and silicon AFM probe in near-contact with a Ag-Au-Ag heterometallic nanorod was illuminated with a focused laser radiation (632.8 nm ,810 nm) and the scattered light is measured as a function of sample position. Different combinations of excitation/detection polarizations reveal different ANSOM images of Ag-Au-Ag heterometallic nanorods that are fully consistent with the excepted local field distributions of plasmon-resonant Ag-Au-Ag nanorods. In addition, we experimentally observe plasmonic coupling between Au and Ag heterometallic nanorods, which is confirmed of ANSOM phase map

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Capturing the vibrational cooling motion of I_2 in CCl_4 via Time-Resolved X-ray Liquidography

이재혁, 이효철

KAIST 화학과

We studied the vibrational cooling motion of hot I_2 in CCl_4 using time-resolved X-ray liquidography. I_2 in CCl_4 were pumped by a picosecond laser pulse, and excited from ground state X to the electronic states A/A'. The excited I_2 molecule recombine geminately. One way is the relaxation from higher vibrational level of X-state to vibrational ground of X-state. The life time of this relaxation in X-state is reported to about 180 ps. Another way is the relaxation in A/A' state. The precise value of the life time of the relaxation in A/A' is now known. However comparison of the potential depth of A/A' and X state, the life time of A/A' state will be expected shorter than that of X state. The other way is the nongeminated recombination of I_2 molecule, which has life time of few ns. Here, we focused on the early relaxation process, the vibrational cooling in X-state and A/A' state. To track these fast vibrational cooling motion, we applied time slicing method which uses only some parts of 100 ps long x-ray pulse in time domain to achieve better temporal resolution of about 10 ps. After deconvolution of experiment data, one can see the atomic distribution change, the change of I-I distance of hot I_2 molecule as a function of time.

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Specific Noncovalent Complexes of Zinc-finger proteins-DNA duplexes detected by ESI-MS

박수진, *조규봉, *오한빈

*서강대 바이오융합학과 *서강대 화학과*

It is well known that the "zinc-finger" family has a strong tendency to bind to its counterpart DNAs through sequence-specific interactions of DNA. In therapeutics, there have been extensive efforts to design a new type of zinc-finger proteins and also to develop an analytical method which can facilitate the screening of the specific recognition of the zinc-finger proteins to DNA duplexes. In the present study, the main target of the screening is to find a zinc-finger protein which show the optimal binding affinity to the targeted DNAs using ESI-MS. DNA binding domains of two peptides, Sp11 and CF2-II, and two DNA sequences (one with a preference for Sp11, 5'-GGGGCGGGGC-3'/ 3'CCCCGCCCCG-5', and the other for CF2-II, 5'-GTATATATA-3'/3'-CATATATAT-5') were selected as a model system to investigate the utility of ESI-MS in detecting sequence-specific peptide-DNA noncovalent complexes. When a mixture of Sp11 and DNA duplex of 5'-GGGGCGGGGC-3'/ 3'CCCCGCCCCG-5' was electrosprayed, a noncovalent complex of Sp11-the GC-rich DNA duplex was observed in a high abundance. This indicates that a Sp11 peptide has a strong affinity to the DNA duplex of 5'-GGGGCGGGGC-3'/ 3'CCCCGCCCCG-5'. The specificity of noncovalent complexes was confirmed by the fact that the noncovalent peak abundance was much higher when a Zn2+ is added. As a negative control, we further examined complexes of Sp11 and DNA duplex of 5'-GTATATATA-3'/3'-CATATATAT-5'. Indeed, the abundance of Sp11 and the AT-rich DNA duplex was much weaker than that of Sp11 and the GC-rich DNA. Instead, CF2-II showed a strong binding affinity to 5'-GTATATATA-3'/3'-CATATATAT-5' duplex. In the poster, we will discuss further experimental details.

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Excitation Energy Migration Processes in Self-assembled Porphyrin Boxes Constructed by Conjugated Porphyrin Dimers

김표상, *Akihiko Tsuda, 김동호

*연세대 화학과 *Kobe University*

Recently, a variety of molecular assemblies as bio-mimic models of natural photosynthetic systems have been synthesized.1,2 Especially, conjugated porphyrin oligomers are highly attractive as building block elements for artificial light harvesting complex, because the linkers have extended conjugation between porphyrin units resulting in low-energy and strong electronic transition of Q bands, which provide enhanced solar spectral absorption and efficient excitation energy hopping (EEH) processes. In this work, we have investigated the EEH processes occuring in the self-assembled zinc(II) porphyrin boxes such as B1, B2, and B4 which are composed of mono-, di-, tetra-alkynylene-bridged porphyrin dimers, respectively. Particularly, alkynylene-linkers allow rotational conformational heterogeneity, which leads to two kinds of self-assembled porphyrin boxes constructed by planar and orthogonal conformers. It was found that the EEH processes occur in the S1 states with the EEH times of 2 ps in all boxes constructed by planar conformers and 12 ps and 8 ps in B2 and B4 constructed by orthogonal conformers, respectively, based on the exciton-exciton annihilation analyses monitored by power-dependent femtosecond transient absorption. According to the calculated Föster energy transfer rate and the observed magnitude and direction of transition dipole moments, increased alkynylene-bridge length leads to the formation of exciton partially localized on porphryin monomer, which result in similar EEH times of all boxes constructed by planar conformers. The dihedral angle of 90 degree provides relatively weak conjugation between porphyrin units, which induces exciton localized state that causes slower EEH times of boxes constructed by orthogonal conformers than that of boxes by planar ones. In conclusion, we suggest that self-assembled zinc(II) porphyrin boxes such as B1, B2, and B4 can be good candidates to realize and control the energy hopping efficiency by tuning alkynylene-bridge length and dihedral angle between porphyrin moieties for artificial light harvesting complexes .

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Computational Study on the Hydrolysis of Pyrophosphates

홍주연, 이제욱, 함시현

숙명여대 화학과

The quantum mechanical calculations were performed to understand the structures and reactions of pyrophosphates with four different charged states (-3, -2, -1, 0). The detailed molecular structures including the equilibrium conformations were carefully investigated and the hydrolysis reaction energies were explored both in gas phase and in aqueous phase. Thermodynamic properties of pyrophosphates in two phases were also discussed by using Gibb's free energy, charge distribution, and dipole moment of pyrophosphates.

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Dispersion-Oriented Soft Interaction in a Frustrated Lewis Pair and the Entropic Encouragement Effect in its Formation

김현우, 이영민

포항공과대 화학과

Frustrated Lewis Pairs (FLPs) are Lewis acid-base pairs with baffled dative bonds between the acid and base parts. FLPs become promising non-metal reagents for activating small molecules such as molecular hydrogen and carbon dioxide. However, the origin of forming FLPs was not investigated clearly. Herein, we present our computational study about the stability of a FLP (tBu$_3$P:B(C$_6$F$_5$)$_3$) induced by the entropic encouragement due to dispersion interactions between phosphines and hexafluorobenzene. Our results indicate that their noncovalent interactions are larger than usual π-π interactions between small aromatic molecules and contribute to entropic effect when a FLP forms. Interestingly, potential surface of tBu$_3$P:B(C$_6$F$_5$)$_3$ pair not only shows this soft interaction, but also implies direct boron-phosphorus interaction conformed by natural bond orbital analysis. Our result will give a useful guideline for researchers who seek to elucidate the mechanism of hydrogen activation performed by FLPs and design other reagents or catalysts based on phosphines and boranes.

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Synthesis and optical properties of CdSSe nanowire using vapor transport method

성태광, 박정희, 장소영, 명윤

고려대 소재화학과

Ternary alloy CdSSe nanowires and nanoribbons were successfully grownthrough a one-step thermal evaporation route using Au as a catalyst. 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 nanoribbons have high-quality single-crystalline nature, and their compositions can be determined as CdS0.9Se0.1and CdS0.75Se0.25,and CdS0.5Se0.5 ans CdS0.25Se0.75 and CdS0.05Se0.95 respectively. The photoluminescence measurements showed very strong band-edge emission for samples, which further demonstrates the single-crystal nature of the as-obtained CdSSe alloys. This finding may be extended for fabricating other composition-tunable 1D ternary alloy nanostructures.

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Ab initio study of predissociative dynamics of XYCZ(X, Y=F, Cl, Br; Z=O, S)

이근혜, 백경구

강릉대 화학과

The excited electronic state of XYCZ(X, Y=F, Cl, Br; Z=O, S) could be a useful target four-atomic system in the study of basic photo-physical and photo-chemical process of polyatomic systems. In order to provide detail information and insights behind the photo-dynamical processes of the XYCZ, the potential energy surfaces (PESs) of the low-lying excited electronic states (S0, T1, S1, S2) of the XYCZ are studied along the three dissociation process (the dissociation of C-X, the dissociation of C-Y, and the dissociation of C-Z), by applying the equation-of-motion coupled cluster singles and doubles (EOM-CCSD) method. Several interesting pre-dissociation processes are disclosed newly, and their aspects are discussed based on some preliminary results of ab initio molecular dynamics (AIMD) as well as the qualitative and quantitative characteristics of the PESs.

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Time-resolved spectroscopic studies on plant leaves

김은철, 김희태, 안태규

성균관대 에너지과학과

Chlorophyll a in plant leaves is suitable for spectroscopic (fluorescence) study because it reflects the conditions of leaves quantitatively. The fluorescence mesurement on living leaves has been developed over more than 30 years. However little is known for the time-resolved fluorescence on leaves. On the other hand, there is a biological question; what happen in the yield of photosynthesis if the differentiation of chloroplast is blocked? In this study, using wildtype *Arabidopsis thaliana* and *arc3* mutant which is geneticaly modified not to make any differentiation in chloroplast, we investigated to measure the fluorescence lifetimes of chlorophyll a to know the effect on photosynthesis along with the size of chloroplasts. We found the lifetime in *acr3* mutants to be longer than that in wildtype. In addition, we have also studied yields of photoprotection in wildtype and *acr3* mutant under high actinic light.

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Comparative Study of Wavepacket Propagation and AIMD method on Early-time Photodynamics

안희선, 백경구

강릉대 화학과

XNO(X=F,Cl), X_2O(X=Cl,Br) 등은 광-동역학의 세부 과정을 자세히 연구하는 좋은 대상들 중 하나이며, 이미 많은 분자동역학 이론 및 실험 연구가 진행되었다. 이러한 3-원자 분자에는 완전한 양자역학 수식으로 wavepacket propagation 을 다루는 방법이 적용될 수 있지만, 보다 일반적인 다-원자 분자를 다루려는 순-이론 분자-동력학(AIMD) 방법에서는 고정-폭-가우시안 함수들의 선형결합을 semiclassical 수식으로 시간-전개하는 방법을 적용할 수밖에 없다. 본 연구에서는 EOM-CCSD 를 사용하는 AIMD 방법과 wavepacket propagation 을 동시에 적용하여 전자-전이 흡수-스펙트럼의 모사하고, 이를 통하여 광-흡수 후 약 ~200 fs.까지의 early-time dynamics 를 다루었다. 두 방법의 결과를 비교하여 AIMD 방법의 프로그램 개발에 필요한 여러 인수들의 최적 값을 조정하였다.

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Systematic study of ab initio methods for TS structure and activation energy of various reactions

김혜미, 백경구

강릉대 화학과

반응물에서 생성물로 진행되는 일반적인 반응 메커니즘은 반응 경로를 따라 하나 혹은 그 이상의 전이구조를 거치게 된다. 실험을 통해서 이러한 전이구조(TS)를 규명하기 매우 어렵기 때문에 이론적인 연구를 통해 전이구조를 탐색하는 것이 화학반응 메커니즘 연구에서 매우 중요하다. 본 연구에서는 여러 ab initio 방법들을 적용하여 몇 가지 반응들의 TS 를 탐색하였다. 이론 방법의 여러 요소들(electron-correlation level, basis sets, DFT functional form, model substitution, etc.)이 각 TS 의 구조와 여기 에너지(activation energy)등에 미치는 영향에 대한 체계적인 분석을 시도하였다. 이를 통하여 각 이론 방법들의 신뢰성, 편의성, 장점과 한계 등을 비교 연구하였다. Metal azido complex 와 organic isothiocyanate 의 반응으로 tetrazole 을 리간드로 가지는 4 개의 isomer 가 생성되는 반응, chlorosilylenoid 와 aldehyde 의 반응으로 dioxasilolane isomer 가 생성되는 반응, 그리고 간단한 생화학 반응을 주 대상으로 연구하였다.

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Controlling the bond length of diatomic molecules with parabollic chirped pulses

장보영, 신석민, *Ignacio R. Sola

*서울대 화학부 *Universidad Complutense de Madrid, Spain*

The Laser adiabatic manipulation of the bond (LAMB) method is a laser scheme that allows enlarging the characteristic bond length of a molecule by preparing a superposition of a bound electronic state and a dissociative electronic state. The word adiabatic refers here to the process by which one avoids increasing the (average) kinetic energy of the nuclei. This is achieved if the nuclear wave function stays basically on the ground state of the potential curve of the coherent superposition of electronic states, also called light-induced potential (LIP).[1] In order to significantly increase the bond length one needs to populate (in fact almost invert the population predominantly anti-bonding orbitals. The bond distance is thus a function of the laser parameters (mainly the carrier frequencies and pulse amplitudes) whichcan be controlled externally.Several LAMB schemes have been proposed in the literature which required at least two laser pulses and involved at least two excited electronic states.[2] In this work we propose an alternative simpler scheme which uses a single pulse with a parabollic chirp, that is, with a qubic dependence of the optical phase. Control on the shape of the laser pulse is also relatively important. We show the underlying mechanism of this novel LAMB scheme and its robustness as well as the possible utility of the method. References:[1] B. M. Garraway et. al., Phys. Rev. Lett. 80, 932 (1998); I. R. Sola et. al., Phys. Rev. Lett. 85, 4341 (2000); B. Y. Chang et. al., J. Chem. Phys., 114, 8820 (2001); B. Y. Chang et. al., J. Chem. Phys. 113, 4901 (2000); B. Y. Chang et. al., J. Chem. Phys. 118, 6270 (2003)[2] B. Y. Chang et.al., Phys. Rev. A 68, 031402 (2003); I. R. Sola et. al., J. Chem. Phys. 119, 10653 (2003); I. R. Sola, Phys. Rev. A 69, 033401 (2004); B. Y. Chang et.al., J. Chem. Phys. 121, 11118 (2004)

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Anomalous Fluorescence from imidazolium based Room-Temperature Ionic Liquids

차선철, *심태규

*서강대 물리학과 *FOM-AMOLF*

Recently anomalous fluorescence phenomenon has been reported from imidazolium based room-temperature ionic liquids. Unlike usual fluorescence from organic chromophores, the fluorescence peak was shown to change following the wavelength of excitation by as much as ~200 nm, extending outside the region in which material absorption was appreciable. We investigated the fluorescence from ionic liquids having 1-butyl-3-methylimidazolium cation at different thermodynamic phases and for samples with varying degree of dilution in water to perturb the bulk structure. These studies together with analysis of the emission spectra by fitting with multiple log-normal functions allowed us to assign features in the spectra, and to determine the mechanism responsible for the unusual fluorescence.

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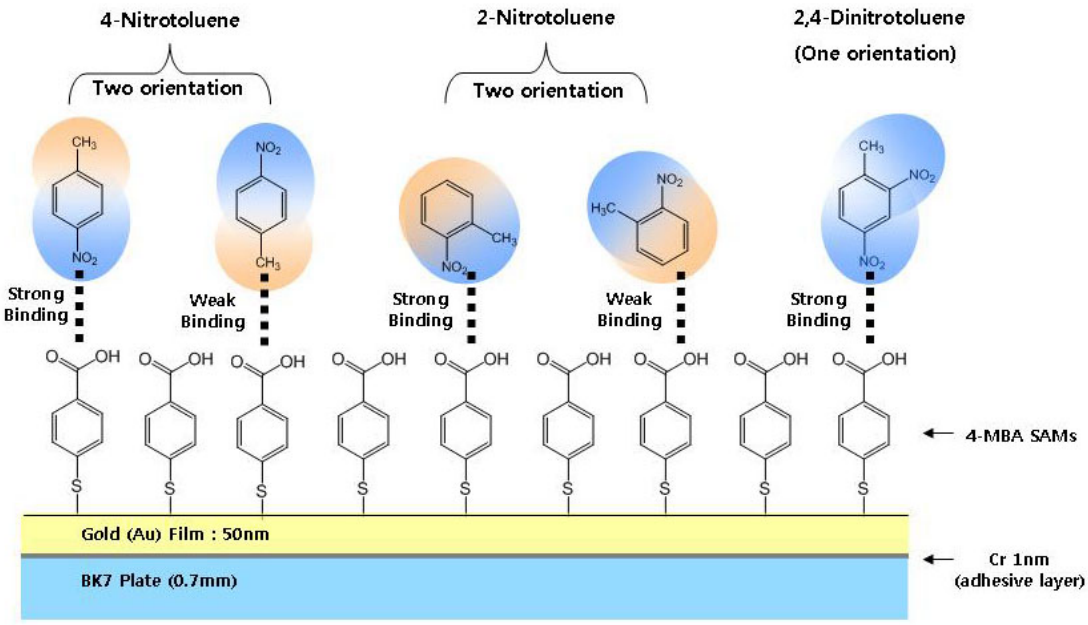
Computational Study of the complexes between nitroaromatic compounds and carboxylic acid-terminated-SAMs for the kinetic analysis of SPR sensorgram

장성우, *양승주, 곽현태, *도영락, 박찬량

*국민대 화학과 *국민대 생명나노화학과*

We studied the interaction complexes between nitroaromatic compounds(nitrobenzene, nitrotoluenes, dinitrotoluenes, trinitotoluene) and carboxylic acid-terminated-SAMs using DFT and ab initio methods. The possible complex conformations were calculated by B3LYP method using 6-31G(d,p) and 6-311++G(d,p) basis set and MP2 method using 6-31G(d,p) basis set. The binding energy(ΔE_{bind}) were calculated applying the basis set superposition error(BSSE) and the zero-point vibrational energies(ΔZPVE) corrections. The results of the calculation revealed that the differences of kinetic behavior between mono nitro-compounds(nitrobenzene, nitrotoluene) and dinitrotoluene(or trinitrotoluene) are due to the dissimilar orientations of the analytes on the homogeneous surface of SAMs. The adsorption/desorption kinetics between nitroaromatic compounds and carboxylic acid-terminated-SAMs were measured by SPR technique and interpreted in terms of the conventional kinetic models in conjunction with the calculation results.



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Molecular Dynamics Simulation Study on the Single Point Mutation Effects on FAS1 Domain 4 Related to Protein Aggregation in Eyes

박미래, 이제욱, 함시현

숙명여대 화학과

The transforming growth factor beta induced protein (TGFBIp, also known as big-h3) is an extracellular matrix protein and it contains four FAS1 domains. It has been reported that mutations on the big-h3 gene, especially R124 and R555 called hot spot, cause protein aggregation and induce a corneal dystrophy in eyes. In this study, we have investigated the effects of single point mutation at the residue R555 on the wild-type 131 residue-long FAS1 Domain 4 composed of six a-helices and six b-sheets by using molecular dynamics simulation. We will mainly focus on the structural characteristics of mutants (R555W and R555Q) comparing with wild-type FAS1 domain 4. The global structures of three proteins are fairly maintained, but local structures of mutants are highly affected by single side-chain mutation.

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Surfaced enhanced fluorescence of rhodamine 6G on mesoporous gold film.

이길용, 김은철, 안태규, *권영욱

*성균관대 에너지과학과 *성균관대 화학과*

형광을 이용한 물질의 특성파악은 광학 소자, 현미경 영상, 생의학적 연구 및 진단 등에 널리 사용되어 지고 있다. 그 중에서 표면증강형광(Surface enhanced fluorescence)은 주로 금과은 나노입자 주변에서 잘 일어난다(Annu. Rev. Phys. Chem. 2007. 58, 267). 방사체(emitter) 주변의 변형과 조절로 전체적인 형광을 효율적으로 산출해 낼 수 있다. 본 연구에서는 로다민 6G (Rhodamine 6G)를 메조동공이 있는 산화 실리콘막 (또는 FTO 나 유리막)에 금을 증착하지 않은 박막과 50 mC 및 145 mC 만큼 증착시킨 박막에 대해서 형광수율과 감소시간을 측정하였다. 그 결과 금을 넣은 경우에 형광수율이 증가한 것을 확인 할 수 있었다. 이를 형광시간분석을 통해 분석하여 비방사성 속도(non-radiative decay rate)의 감소가 형광 수율의 증가에 직접적으로 관여한다는 것을 확인하였다. 반면에 방사성 속도(radiative decay rate)은 거의 변하지 않았다. 이를 통해 향후 보다 나은 형광을 가지는 나노광자소자(nano photonic device)를 개발하기 위한 박막의 설계원리를 제안할 수 있다.

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Effect of Mn doping on enhancement of THz emission in III-V ternary alloy semiconductor nanowires

정경복

고려대 소재화학과

Terahertz (THz) radiation is a promising light source for various important applications such as time-domain THz spectroscopy, THz imaging, and pump-probe dynamics analysis with subpicosecond time resolution. Recently, as a new compact THz generation source, nanostructures have attracted a considerable amount of attention, because of their strong enhancement effect of the surface local field. We observed the terahertz (THz) emission from single-crystalline GaAs-based (GaAs, GaAs0.93Sb0.07, Ga0.92In0.08As) and Mn-doped GaAs-based (Ga0.98Mn0.02As, Ga0.95Mn0.02AsSb0.03, Ga0.94In0.04Mn0.01As) nanowires (NWs), and compared it with each other. Upon their excitation using a Ti-sapphire laser pulse (800 nm), the THz radiation intensities of ternary alloy NWs such as GaAs0.93Sb0.07 and Ga0.92In0.08As are more intense than from GaAs NWs, due to higher absorption and lower effective mass. In addition, the Mn-doping enhances significantly the intensity of the THz emission, which could be attributed to high dc Hall conductivity by the strong influence of the magnetization.

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Three Synthesis Routes of Single-Crystalline PbS Nanowires and Their Electrical Transport Properties

장소영, *송윤미, 김한성, 서영석, 박정희

*고려대 소재화학과 *고려대 소재화학과 태양에너지소재*

Single-crystalline rock-salt PbS nanowires (NWs) were synthesized using three different routes; the solvothermal, chemical vapor transport, and gas-phase substitution reaction of pre-grown CdS NWs. They were uniformly grown with the [100] or [110], [112] direction in a controlled manner. In the solvothermal growth, the oriented attachment of the octylamine (OA) ligands enables the NWs to be produced with a controlled morphology and growth direction. As the concentration of OA increases, the growth direction evolves from the [100] to the higher surface-energy [110] and [112] directions under the more thermodynamically controlled growth conditions. In the synthesis involving chemical vapor transport and the substitution reaction, the use of a lower growth temperature causes the higher surface-energy growth direction to change from [100] to [110]. The high-resolution X-ray diffraction pattern and X-ray photoelectron spectroscopy results revealed that a thinner oxide-layer was produced on the surface of the PbS NWs by the substitution reaction. We fabricated field effect transistors using single PbS NW, which showed intrinsic p-type semiconductor characteristics for all three routes. For the PbS NW with a thinner oxide layer, the carrier mobility was measured to be as high as 10 cm2V−1s−1.

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CdTe Nanoparticles into twist ribbons shapy by Self-Assembly

이광원, 김기섭

충주대 화공생물공학과

The electrical and optical properties of nanoparticles (NPs) and nanowires (NWs) have been extensively studied for use in electronics, photonics, and sensors. Recently, one of the most active areas of research in nanoscience is to develop novel structures of nanomaterials such as nanohelices (NHs), nanosheets (NSs), and hollow nanocrystalls, which open up the possibility of a new generation of advanced materials.Given that the properties of materials largely depend on their unique structure, identification of the key factors in synthesis can be helpful in reaching specific desired shapes. The study on synthesis of NRIs started on the basis of simple hypotheses and modifications of the procedures described. First, the aqueous redissolution step of NPs obtained after precipitation of the original stable dispersion by methanol treatment proceeds under ambient light, because light might cause some defect such as truncation. Second, the ratio of thioglycolic acid (TGA) to Cd2+ is reduced at the synthesis step of CdTe NPs, because we can readily predict that highly photoluminescent (PL) CdTe nanocrystals (NCs) will be obtained at reduced ratios.Furthermore, the excess stabilizers in the CdTe solutions and the stabilizers on the NP surface can be efficiently removed at reduced ratios.

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Studies of Proton-bound Cytosine, Guanine Homo and Hetero DNA Base pairs in the gas-phase: Infrared Photodissociation Spectroscopy (IRPD) and DFT Calculations

성연미, *안화근, **박수진, ***한상윤, 오한빈

*서강대 화학과 *서강대 물리학과 **서강대 바이오융합학과 ***한국표준과학연구원 나노바이오융합연구단*

Extensive studies, both experiments and theory, have been performed for neutral DNA base pairs. However, a little experimental effort has been made for proton-bound DNA base pairs, which may have different binding interactions or structures. 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 6-3111+G(d,p) and 6-3111+G(2d,p). We measured the degree of photodepletion of guanine (G), cytosine (C) homo- and hetero-dimers as a function of irradiating IR laser wavelength. The probed wavelength region was 2640–3761 cm-1 which corresponds to C-H/N-H/O-H stretching vibrational modes within dimeric complexes. In three IRPDS spectra for GG, CC, and GC dimers, a couple of photodepletion peaks were observed, which presumably correspond to vibrational features of the above DNA base dimers. These vibrational spectral features were compared with the DFT calculation results, which showed a good agreement to each other. In the poster, we will show the structures of the DNA base pairs obtained by the DFT calculations and further show the details of the experiments.

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Preparation and Optical Properties of Ir(III) complexes with β-diketone ligands

이효성, 강준길

충남대 화학과

Phosphorescent iridium(III) complexes, Ir(DFPP)2(β-diketone) (DFPP = 2-(2,4-difluorophenyl)pyridine) are synthesized and their optical properties are investigated. β-Diketone ligands used as ancillary ligands in this study are acetylacetone(acac), 1-(2-theonyl)-3,3,3-trifluoroacetone(TTFA), 4,4,4-trifluoro-1-phenyl-1,3-butanedione(TFPB), 4,4,4-trifluoro-1-(2-furyl)1,3-butanedione(TFFB), 4,4,4-trifluoro-1-(2-naphthyl)-1,3-butane dione(TFNB). The optical properties of Iridium(III) complexes are very dependent on β-diketone ligand. In this presentation, the optical properties of the iridium(III) complexes will be comprehensively discussed.

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Noble metal (Au, Ag, and Pt) nanocrystals and their Cu2S nanocrystals hybrid nanostructures.

박기영, 조용재, 김창현, 김한성, 박정희

고려대 소재화학과

Photocatalysis has attractive potential applications in the conversion of solar energy into chemical energy (e.g., the production of H2). Recent research demonstrated the improved photocatalytic activity of semiconductor-noble metal nanocrystal (NC) hybrid nanostructures toward the degradation of organic molecules. The electron transfer from the conduction band of the semiconductor sensitizer to that of noble metal NC can lead to efficient and longer charge separation by minimizing the electron-hole recombination. However, the charge separation abilities of the NC sensitizers with noble metal nanocrystals such as Au, Ag, and Pt were rarely compared, although this information would provide valuable information on the mechanism of the photocatalytic redox reaction. The present work reports the size-controlled synthesis of Au, Ag, and Pt NCs and their Cu2S NCs hybrid nanostructures, which were prepared by the in-situ solvothermal method. Their photocatalytic abilities of hybrid nanostructures toward the dioxane and methylene blue were compared under visible light irradiation, providing the relative efficiency of charge transfer.

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On-chip immunoasaay using surface-enhanced Raman scattering of hollow gold nanospheres

전향아, *이상엽, 정은수, 주재범

*한양대 바이오나노공학과 *한양대 응용화학과*

A quick and reproducible surface-enhanced Raman scattering (SERS)-based gradient optofluidic sensor, using hollow gold nanospheres (HGNs) and magnetic beads, has been developed. A novel microfluidic sensor with functional internal structures has been designed and fabricated. This sensor is composed of three compartments consisting of the gradient channel that serially dilutes the target marker, the injection and mixing area of antibody-conjugated hollow gold nanospheres and magnetic beads and the trapping area of sandwich immunocomplexes using multiple solenoids. Quantitative analysis of a specific target marker is performed by analysing its characteristic SERS signals. This SERS-based gradient optofluidic sensor can replace the set of microwells or microtubes used in manual serial dilutions that have been traditionally used in ELISA-type assays. According to our experimental results, the limit of detection for rabbit immunoglobin (IgG) is estimated to be 1–10 ng/mL. Furthermore, the assay time took less than 25 min, including washing and optical detection steps. 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.

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Synthesis and luminescence properties of Eu(II) complexes

김현준, 강준길

충남대 화학과

Europium(II) complexes, Eu(beta-diketone)$_2$ and Eu(phthalic acid)$_2$, are synthesized and their photophysical properties are investigated. beta-Diketones used in this work are 4,4,4-trifluoro-1-(2-furyl)-1,3-butanedione, 4,4,4-Trifluoro-1-phenyl-1,3-butanedione and dibenzoylmethane. The synthesized Eu(II) complexes are confirmed with EA, ICP and TGA. The Eu(II) complexes, excited at UV, produce blue luminescence. Luminescence properties, such as emission and excitation spectra, quantum yield and decay time, are investigated in this study.

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Synthesis and chracterization of green phosphors for white light emitting diode

김현준, 강준길

충남대 화학과

Several sulfide phosphors were synthesis and their luminescence properties. $(Zn_{(1-x-y)}Sr_xMg_y)_aGa_bY_cS_{5+3c/2}$: pEu^{2+}, qRe^{3+}, rF^- as green phosphor were synthesize solid state method. starting materials ZnO, $SrCO_3$, MgO, Ga_2O_3, Y_2O_3, Sulfur, NH_4F and Eu_2O_3. Re was lanthanide element. Thermal treatment was carried in electric furnace for 3 hour at 850℃ under N_2/H_2 reducing atmosphere. luminescence property of . $(Zn_{(1-x-y)}Sr_xMg_y)_aGa_bY_cS_{5+3c/2}$: pEu^{2+}, qRe^{3+}, rF^- was investigated as a function of x, y, a, b, c, p, q. The maximum intensity was x=0.6, y=0.1, a=2, b=2, c=2, p=0.21, q=0.12 and Re=Dy.

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Growth of Various ZnO Nanocrystals by Chemical Vapor Transport

이슬기, 최명룡

경상대 화학과

In this study, various ZnO nanocrystals were grown onto the ZnO nanofilms, prepared on silicon wafer substrates by a sol-gel method by a chemical vapor transport (CVT) method without catalysts. The growth conditions were adjusted by changing temperatures of the substreate and the pressures of the carrier gases. The structural and morphological properties of the nanocrystals were characterized by X-ray diffraction (XRD) and field emission scanning electron microscope (FE-SEM). The optical properties of the nanocrystals were investigated by photoluminescence (PL) and UV-vis spectroscopy.

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Synthesis of Au-Cu_2S Nanocrystals and Their Visible-Light-Driven Photocatalytic Activity Toward Oxidation of 1,4-Dioxane

김윤희, 박기영, 명윤, 장동명, 박정희

고려대 소재화학과

Au-Cu_2S core-shell NPs were synthesized for the first time using the in-situ solvothermal growth of Cu_2S on Au. The average sizes of the Au-Cu_2S and Au core NPs were 7 and 3 nm, respectively. The photocatalytic degradation of 1,4-dioxane was achieved using the free Cu_2S, CdS, and PbS NPs under visible light irradiation, with the highest degradation yield being observed for the Cu_2S NPs, viz. 60 % after 5 h. The incorporation of the Au core into the NPs significantly decreases their efficiency to 30 %. The comprehensive data analysis suggests the excellent photocatalytic reduction activity of the Cu_2S NPs toward the generation of H_2O_2, which leads to the oxidative degradation of dioxane. Their photocatalytic reduction power would be suppressed as the Au core withdraws the electrons from the Cu_2S shell.

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DNA-Functionalization of Visible Light-Sensitive ZnO Nanowires: Optical Characterization

이주란, 윤민중

충남대 화학과

Single crystalline visible light-sensitive ZnO nanowires were functionalized with single-stranded DNA for the development of biosensors. Aminopropyltriethoxysilane (APTES) as a linker, APTES-bound ZnO nanowires were found to depends on various APTES addition times, as confirmed by SEM, XPS and AFM. Onto the APTES-bound ZnO nanowires, 16 bases 5'-aldehyde-modified DNA (OCH-ssDNA) was immobilized. The photoluminescence (PL) spectra of DNA-functionalized ZnO nanowires were measured upon excitation with 415 nm laser beam, demonstrating that the optical properties of ZnO nanowries were changed while the DNA was conjugated. These results indicate that the PL properties of the DNA functionalized ZnO nanowires are very useful to analyze the complementary DNA by visible light excitation.

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Synthesis and Characterization of Water-Soluble fluorene based Polymer as an Electron Injecting Materials in Polymer Light-Emitting Diodes.

안호익, 최종완, 김낙중

한양대 화학과

For more than a decade, polymer light-emitting diodes (PLEDs) have attracted continuous attention because of their many advantages, such as low costs, easy processability and low drive voltage. And PLEDs have application potential in large-area solid state lighting source and backlights for liquid-crystal displays. In this study, we synthesized and characterized fluorene based conjugated polymer by palladium-catalyzed Suzuki coupling reaction. The conjugated polymers were characterized by using the UV-vis, PL(Photoluminescence) and CV(cyclic voltammetry). And the HOMO and LUMO energy level of the polymer was calculated by using the VAMP-AM1 method in the material studio 4.1 program.

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Synthesis of GaAs1-xSbx, Ga1-yMnyAs1-xSbx nanowires and their magnetic properties.

공강준, 정찬수, 김한성, 박정희

고려대 소재화학과

GaAs1-xSbx and Ga1-yMnyAs1-xSbx nanowires were synthesized with finely controlled Sb and Mn contents (x = 0, 0.03, 0.05, 0.06 and 0.09 and y = 0, 0.01, 0.02) by the vapor transport method. They consisted of single-crystalline zinc blende GaAs nanocrystals (avg. diameter = 60 nm) grown along the [111] direction. The Sb doping increases the lattice constant, most significantly at x ≈ 0.07. X-ray photoelectron spectroscopy revealed that as the Mn and Sb content increases, the binding energy of Ga 2p and As 2p shifts to a higher energy, which can be correlated with the hybridization between the Mn2+ ions and the holes. X-ray absorption spectroscopy and X-ray magnetic circular dichroism confirmed that the Mn2+ 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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Preparation and luminescence properties of oxynitride phosphors for light-emitting device

오성일, 유진호, 강준길

충남대 화학과

Several oxynitride phosphors were synthesis and their luminescence properties.

대한화학회 THE KOREAN CHEMICAL SOCIETY

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Synthesis of Pt Nanoparticles by Laser Ablation and Their Catalytic Activities using Polymeric Stabilizers

이승준, *한상우, 최명룡

*경상대 화학과 *KAIST 화학과*

The effect of polymeric stabilizers on the catalytic activity of Pt nanoparticles for an electron transfer reaction between $Fe(CN)_6^{3-}$ and $S_2O_3^{2-}$ was investigated. Pt nanoparticles were prepared by laser ablation of Pt plate in water, and then stabilized with typical stabilizing polymers such as poly(vinyl pyrrolidone) (PVP), poly(vinyl sulfate) (PVS), and polyethylenimine (PEI). The catalytic reaction proceeds much faster with PEI-stabilized nanoparticles than PVP- or PVS-stabilized particles. The activity of nanoparticles also highly depends on pH and polymer concentration. These clearly demonstrate that the net charge of the stabilizers plays a decisive role for the nanoparticle-mediated electron transfer between charged reactants.

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Growth of ZnO Nanorods by a Hydrothermal Method

정현진, 이슬기, 최명룡

경상대 화학과

ZnO nanorods were grown by a liquid phase epitaxial growth on silicon wafers deposited with a ZnO thin film as the seed layer, which is prepared by a sol-gel method and a spin coating technique. The growth behavior of the well-aligned ZnO nanorods on the seed layer films were adjusted by gel composition ratios, spin-coating process, precursory solution volume, temperature and time. The structural and morphological properties of the resulting ZnO nanorods were characterized by field emission scanning electronic microscope (FE-SEM), X-ray diffraction (XRD) and Ultraviolet-visible spectroscopy (UV-vis).

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특이값 분해 분석을 이용한 용액상 단백질의 구조 동력학 분석

Structural Analysis of Proteins Dynamics in Solution Using the Singular Value Decomposition (SVD) Analysis

김종구, 김영민, *왕기영, **이재혁, **이효철

*KAIST 화학과 *KAIST 나노과학기술대학원 **KAIST 화학과*

Three-dimensional structure of proteins is directly related to the function of the proteins. So, it is essential to study about the structure of proteins. We can track protein structural changes in solution with time-resolved wide-angle X-ray scattering (TR-WAXS). Because the condition of the TR-WAXS which is proceeded in solution is similar with biological conditions, studies with TR-WAXS in solution can be a good approach to protein functional studies. Here we will introduce an example of analyzing TR-WAXS data with the singular value decomposition (SVD) analysis. In linear algebra, the singular value decomposition (SVD) is an important factorization of a rectangular real or complex matrix, with many applications in signal processing and statistics. A matrix to be analysed is made by scattering intensities with scattering angle at various time delays. The column vectors are scattering intensities with scattering angles at fixed time delay and the row vectors are scattering intensities with time at a fixed scattering angle. From the SVD calculation, we can get the left singular vectors and the right singular vectors and the singular values. Also, left singular vectors are set of basis vectors of the column vectors of the original matrix and right singular vectors are set of basis vectors of the row vectors of the original matrix. Because the original matrix contains information of changes in scattering intensity with time as row vectors, we can infer structural changes of proteins in process of the reactions by analysing the right singular vectors. TR-WAXS data was measured for horse myoglobin (Mb) and the SVD analysis was conducted from this data. Mb is a heme protein that carries small ligands like O2, CO and NO in muscles and can be considered as a subunit of hemoglobin. The laser pulse induces photolysis of the CO ligand from the heme of the protein and it accompany structural changes. As the ligand is detached from the heme, well-

known R to T transition (from relaxed form to tense form) is involved inside the Mb. We carry out the SVD analysis and get the information about reaction intermediates and reaction kinetics of Mb photolysis.

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Composition control in chemical vapor transport grown $In_XGa_{1-X}As$ nanowires

정찬수, 공강준, 김한성, 박정희

고려대 소재화학과

Ternary composition $In_XGa_{1-X}As$ nanowires (NWs, 0< x $_XGa_{1-X}As$ NWs, using the $MnCl_2$ vapors. The magnetization measurement revealed that these Mn doped InXGa1−XAs nanowires exhibited ferromagnetic behavior, which is stronger than that of GaAs NWs. X-ray absorption spectroscopy and X-ray magnetic circular dichroism confirmed that the Mn^{2+} ions substitute into the tetrahedrally coordinated Ga or In sites

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REMPI and UV-UV Double Resonance Spectroscpy of Jet-Cooled Indole

민아름, 이승준, *김성근, 최명룡

*경상대 화학과 *서울대 화학부 & 서울대 생물물리 및 화학생물학과*

Indole as a precursor of tryptophan has an important intrinsic property for its enormous biological activities in biological systems. We measured the excitation spectra of indole monomer using one color resonant two photon ionization(R2PI) in the spectral range of 35087-35842cm^{-1}. We observed the origin transition, the most intense peak at 35245cm^{-1}. By fixing the probe laser at the 0-0 origin band and scanning the hole burning laser, we have obtained a UV-UV double resonance spectrum of indole. In the near future, we will interrogate the structural information of indole dimers with resonance-enhanced multiphoton ionization (REMPI) and UV-UV double resonance spectroscopic methods.

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Fabrication and photocatalytic activity of novel metal / TiO_2 nanofiber composites

오승임, 최경훈, 임지은, 왕강균, 김용록

연세대 화학과

The mesoporous TiO_2 nanofibers are fabricated by using sol-gel method within a nanoporous alumina membrane. Photocatalytic functionality of the composite nanofibers is investigated for the properties induced by the size and quantity of the deposited precious novel metal nanoparticles. The composite materials were prepared by deposition-precipitation with $HAuCl_4$ solution as modified catalyst, and sol-gel reaction with titanium(IV) isopropoxide. The photocatalytic activities are evaluated by the degradation of organic dye in an aqueous solution. The activity of the modified catalyst was estimated to be 30% higher than that of the pure mesoporous titania nanofiber.

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LIF, REMPI and UV-UV Double Resonance Spectroscopic Studies of Jet- Acetaminophen

김유식, 이승준, *이상학, **김성근, 최명룡

*경상대 화학과 *서울대 화학부 **서울대 화학부 & 서울대 생물물리 및 화학생물학과*

In this work, we present the conformational structures and photochemistry of jet-cooled acetaminophen, widely used as a pain reliever and fever reducer, studied by resonant enhanced multi-photon ionization (REMPI), UV-UV double resonance and laser induced fluorescence (LIF) spectra in the gas phase. Conformational characterizations for acetaminophen will be presented with an aid of spectroscopic techniques and DFT B3LYP calculations. Experimental techniques, vacuum chambers, with supersonic expanded molecular beams, electronics and a pulsed Nd:YAG based tunable laser system, will also be presented.

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Synthesis and property of photoluminescence of schiff base complex

정용광, 장지아, 강준길

충남대 화학과

Disalicylidene-1,2-ethanediamine Schiff-base ligand, N2O2, as a tetradentate chelate was prepared from salicylaldehyde and ethylenediamine. Trivalent lanthanide complexes with homoleptic N2O2 and with mixed N2O2 and phen (1,10-phenanthroline) were prepared and their luminescence properties were investigated. It was found that the energy transfer from N2O4 to Eu(III) results in highly effective sensitized red luminescence. The sensitized red luminescence from Eu(III) complexes were characterized in terms of excitation and quantum yield.

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ROS Effective Functional Nanolayer Coatings on NiTi Alloy

최경훈, 신언필, 왕강균, 김봉진, 오승임, 임지은, *김환규, 김용록

*연세대 화학과 *고려대 신소재화학과*

Application of Reactive Oxygen Species (ROS) is a promising approach for killing microorganism and especially for the inactivation of antibiotic-resistant strains. This work describes a method of ROS generating nanolayer coating on NiTi alloy which shows a good biocompatibility. The ROS generating nanolayer coatings were prepared by a simple surface modification process. The microstructure and the elemental and phase composition of the coating were investigated by scanning electronmicroscopy (SEM), energy dispersive X-ray spectrometer (EDS), and X-ray diffraction (XRD). Result of this study shows that the PtCP functional nanolayer coating is composed of many perpendicular nanosheet structures. The ROS generation efficiency of the PS being chemically bonded on these nanosheets is detected by using the decomposition of 1,3-diphenyl-isobenzofuran.

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Characterization of ZnO/Zn Nanoparticles Grown by Liquid-Phase Pulse Laser Ablation (LP-PLA).

안아름, 이승준, 최명룡

경상대 화학과

Size and composition controlled ZnO/Zn nanoparticles were prepared by laser ablation of a Zn metal plate in a various solvents with different surfactants. A pulsed Nd:YAG laser was used to produce the nanoparticles. The structural and morphological characterization was conducted by X-ray diffraction (XRD) and field emission scanning electron microscope (FE-SEM). A detailed study of Tthe optical behaviors of the nanoparticles investigated by UV-Vis will be presented.

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Photoelectron imaging study of photoionization of methylamine isotopomers via the predissociative excited state

이정묵, 안두식, 김상규

KAIST 화학과

We present photoelectron images resulting from the photoionization of various methylamine isotopomers (CH_3NH_2,CH_3ND_2 and CH_3NHD) with various selected vibrational states. $NH(D)_2$-wagging(ν_9), CH_3-rocking(ν_7) and their combination bands(ν_7+ν_9) were selected as the specific vibrational states on the predissociative well in S_1 state. There were many distinct peaks in photoelectron images and it seems that they are initial vibration, its combination band with $NH(D)_2$ symmetric stretching vibration and $NH(D)_2$ scissoring mode. There is no specific vibraional mode dependence on features of photoelectron kinetic energy distributions. It seems that wagging mode(ν_9) and rocking mode(ν_7) of methylamine are almost orthogonal each other on N-H reaction coordinate.

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Hydrogen uptake efficiency of mesoporous carbon nanofiber and its structural factors to determine the uptake efficiency

임지은, 오문현, 김용록

연세대 화학과

Carbon is one of the most widely used as industrial adsorbent which has the advantage of their hydrophobic surface, high specific area, good thermal stability, and low specific weight. In this study, the fabricated mesoporous carbon nanofibers were tested for their capacities of hydrogen storage. The mesoporous carbon nanofibers (MCNF) were synthesized by using a template of mesoporous silicate nanofibers within anodic aluminum oxide (AAO) film and furfuryl alcohol for the carbon source at the carbonization temperatures (600, 900, 1200 °C). Due to the easy controllability of pore size and thickness of AAO nanochannels, the diameter and length of MCNF can be custom synthesized for a specific application. The hydrogen uptake capacity which sensitively depends on the above factors was measured at 77 K and ambient pressure of 0.1 MPa and the MCNF-1200 with the largest BET area and pore volume provided the highest hydrogen strorage of 0.74 wt.% among the MCNFs investigated in this study.

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Electrochemical biosensor for the detection of estrogen hormone by immobilized estrogen receptor

LIJING, 김병건, 임지은, 한지훈, 이원용, 김용록

연세대 화학과

An electrochemical impedance immunosensor for the detection of estrogen by estrogen receptor at an Au electrode. Detection of estrogen which is one of steroid hormones has intensively been investigated due to its functionalities of estrus arising and cancer causing elements. In this study, the immunological reaction between the hormone and its receptor is applied for the detection of estrogen, which enables high selectivity. Moreover, since EIS (Electrochemical Impedance Spectroscopy) method is applied, the highly sensitive detection becomes possible in a wide range of concentration. In order to fabricate the electrode covalently bonded with estrogen receptor, the modified electrode which was utilized for the molecules including thiol groups and carboxyl groups.The cross linkers are involved to form a solid covalent bonding to estrogen receptor. The surface ohmic resistivity is measured at each step of fabrication by electrochemical impedance method and intermolecular bonding energy is monitored by XPS (x-ray photoelectron spectroscopy) at each step.

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The theoretical study of HOOO-H_2O complexes

이주영, 김승준

한남대 화학과

The hydrotrioxy (HOOO) radical has been known as key intermediate in atmospheric chemistry, where the hydrogen-oxygen system is significantly acted. It is important to note that HOOO radical can be stabilized by formation of a complex with water in the atmosphere. The structures, thermodynamical stabilities, and spectroscopic properties of HOOO-H_2O complexes have been investigated at the B3LYP level of theory using the aug-cc-pVTZ basis set. The equilibrium structures and relative energies for the possible local minima have been fully optimized and the harmonic vibrational frequencies have been predicted to confirm the local minimum and to correct the zero-point vibrational energy.

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Development of fluorescence-SERS dual modal nanoprobes for smart cancer diagnosis

이상엽, *전향아, 고주희, *주재범

*한양대 응용화학과 *한양대 바이오나노공학과*

This paper describes a highly sensitive optical imaging technology using dual-modal metal nanoparticles for cellular imaging or biomedical diagnostics. Fluorescence microscopy is a well-known imaging technique which provides a specific protein distribution inside cells. However, most of currently available fluorescent organic dyes have relatively weak emission intensities and they are also photo-bleached quickly. In order to resolve this problem, more sensitive and stable probes are still needed. In the present work, dual modal nanopronbes, which can be used for both the Surface-enhanced Raman scattering (SERS) and fluorescence detections, have been developed. SERS detection is a powerful analytical technique that allows ultra-sensitive chemical or biochemical analysis in terms of unlimited multiplexing and single molecule sensitivity. Combining advantages of fluorescence and SERS allow these dual modal nanostructures to be used as powerful probes for a novel biomedical imaging.

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Computer Simulation Studies of the Correlation between Cell Degenerative Diseases and Neurofilaments

김성훈, 장락우

광운대 화학과

According to recent research in neurobiology, neurofilaments are tied to the cell degenerative diseases such as multiple system atrophy or multiple sclerosis and several experiments found that some of these diseases are accompanied by the change in the ratio of three different neurofilament sidearms representing NF-L (light), NF-M (medium), and NF-H (heavy). Therefore, there have been some speculations that neurofilaments may be used as the biomarkers of these diseases.To investigate the correlation between the ratio of neurofilament sidearms and various cell degenerative diseases, we have performed Monte Carlo simulations using a coarse-grained model of a neurofilament brush, which has been successfully applied to the study of the structural properties of neurofilaments.

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Kinetic Study of DNA Double Strand Breaking by 3-color Alternating Laser Excitation Fluorescence Resonance Energy Transfer

권지웅, *정지원, *이상학, **김성근

*서울대 생물물리 및 화학생물학과 *서울대 화학부 **서울대 화학부 & 서울대 생물물리 및 화학생물학과*

UV irradiation often induces DNA damage through such diverse mechanisms as thymine photodimerization, DNA base deletion, and double strand breaking (DSB). We investigated the kinetics of DSB by using 3-color Alternating Laser Excitation Fluorescence Resonance Energy Transfer. We attempted to explain the different DSB kinetics measured between the AT-only and GC-only DNA sequence by the electron affinity of the DNA bases or the efficiency of electron transfer from the pre-solvated electron to the base, in view of the known solvated electron mechanism for DSB. We also varied the AT/GC-ratio and found that it affects the DSB kinetics rather strongly.

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발표분야: 물리화학
발표종류: 포스터, 발표일시: 목 15:00~17:00

UV-induced DNA Double Strand Breaking Studied by Fluorescence Correlation Spectroscopy

정지원, *권지웅, **김성근

*서울대 화학부 *서울대 생물물리 및 화학생물학과 **서울대 화학부 & 서울대 생물물리 및 화학생물학과*

We investigated UV-induced breaking of dsDNA by generating solvated electrons as an active damaging agent using pulsed femtosecond UV laser. Under the same chemical and optical conditions, the correlation curve was significantly different between AT-only and GC-only DNA sequence. We also found that the AT-only DNA sequence was damaged more easily than the GC-only DNA sequence. In addition, we varied the GC/AT-ratio of the sequence to investigate the sequence-dependent kinetics of dsDNA damage and its mechanism.

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Water disinfection effect of reactive oxygens generated by photofunctional nanoporous membrane

왕강균, 하재욱, 김봉진, 민경명, 김용록

연세대 화학과

Water disinfection with nanomaterials has been a subject of extensive studies due to there potential applications environmental and health care industries. In this work, we report fabrication of the photo-functional nanoporous memebrane and there photophysical properties estimated with various spectroscopy method. The fabricated photofunctional nanoporous membrane were applied for the elimination of health hazards.

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Infrared photodissociation spectroscopy of the ternary cluster cation of aniline-water-methanol and the special investigation of the N-H stretching vibrations of the ternary cluster cation.

MD.ALAUDDIN, 신승근, 송재규, 박승민

경희대 화학과

Abstract The infrared photodissociation spectrum of aniline-water-methanol cluster cation has been measured in the 2600-3900 cm-1 region. Six absorption bands have been observed at 3017, 3227, 3423, 3647, 3674 and 3725 cm-1, which have been assigned to the symmetric stretching vibration of NH in the aniline ion, anti-symmetric stretching vibration of NH in the aniline ion, free NH stretching vibration of the aniline ion, symmetric stretching vibration of OH of water, free OH vibration of methanol and anti-symmetric stretching vibration of OH of water, respectively. It has been found that an infrared photon can decompose the cluster cation AWM+ into photofragments in two different reaction paths: AWM+→AM+ + W and AWM+ → AW+ + M (A: aniline, W: water, M: methanol). The branching ratio (AW+/(AM+ +AW+)) has been determined to be 0.036±0.003 for the symmetric NH (3017 cm-1, hydrogen bonded to methanol) stretching vibration of aniline ion and others are so far from this band. From this observation, it is suggested that the ultra-fast energy transfer has been occurred from the symmetric NH stretching mode to the intermolecular vibration through hydrogen bond rather than anti-symmetric NH stretching mode.

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발표종류: 포스터, 발표일시: 목 15:00~17:00

Competitive Ion-Molecule Reactions within $V^+(CH_3COOCH_3)_n$ Clusters

폴다바브라타, 김태규, *정광우

*부산대 화학과 *원광대 화학과*

A laser-ablation/molecular beam method have been used to investigate the competitive insertion reactions of V^+ within $V^+(CH_3COOCH_3)_n$ heteroclusters. The mass spectrum exhibited peaks corresponding to two types of reaction products: (a) V^+-containing clusters and (b) VO^+-containing clusters. The promising $VO^+(CH_3COOCH_3)_n$ clusters formation was exclusively dominated by the oxidative addition reaction of V^+ with methyl acetate. The observation of this product ions are well understood on the basis of a C=O and C-O (ester) insertion reaction via complex I and complex II, respectively. In case of complex I, product formation occurred followed by H atom transfer and CH_2CHOCH_3 elimination. In contrast to the complex I, methyl migration and acetone elimination is the plausible pathway for complex II. Density functional theory calculations were performed to rationalize the reaction pathways and energetics of the proposed mechanism.

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Theoretical investigation for the molecular structures and interaction energy for complexes of $C_6H_6^+$-$(H_2O)_n$ (n=1-5)

김시조, 김승준

한남대 화학과

The intermolecular interaction between aromatic molecules and water plays a key role for many biophysical phenomena[1]. The benzene-water, Bz-H_2O has been well known that π electrons on a conjugated system can accept hydrogen to form a weak hydrogen bond, that is, so called π-hydrogen bond[2]. The benzene-water cation complex, $[Bz\text{-}H_2O]^+$ is mainly bound by charge-dipole interaction. The global minimum structures of the $[Bz\text{-}H_2O]^+$ have been investigated using *ab initio* and density functional theory(DFT) with large basis sets. The highest levels of theory employed in this study are B3LYP/aug-cc-pVTZ for geometry optimization and MP2/aug-cc-pVTZ for interaction energy. The harmonic vibrational frequencies and IR intensities are also determined at the B3LYP/aug-cc-pVTZ level of theory to confirm whether the structure of water complexes is affected by the presence of benzene.

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Femtosecond soft x-ray spectroscopy of solvated transition metal complexes

조하나, 김태규

부산대 화학과

We report the first femtosecond soft x-ray spectroscopy of solvated transition-metal complexes. Structural dynamics mediate ultrafast spin-state conversion and symmetry-specific valence-charge localization. This study demonstrates the unique potential of ultrafast soft x-ray spectroscopy in solutions

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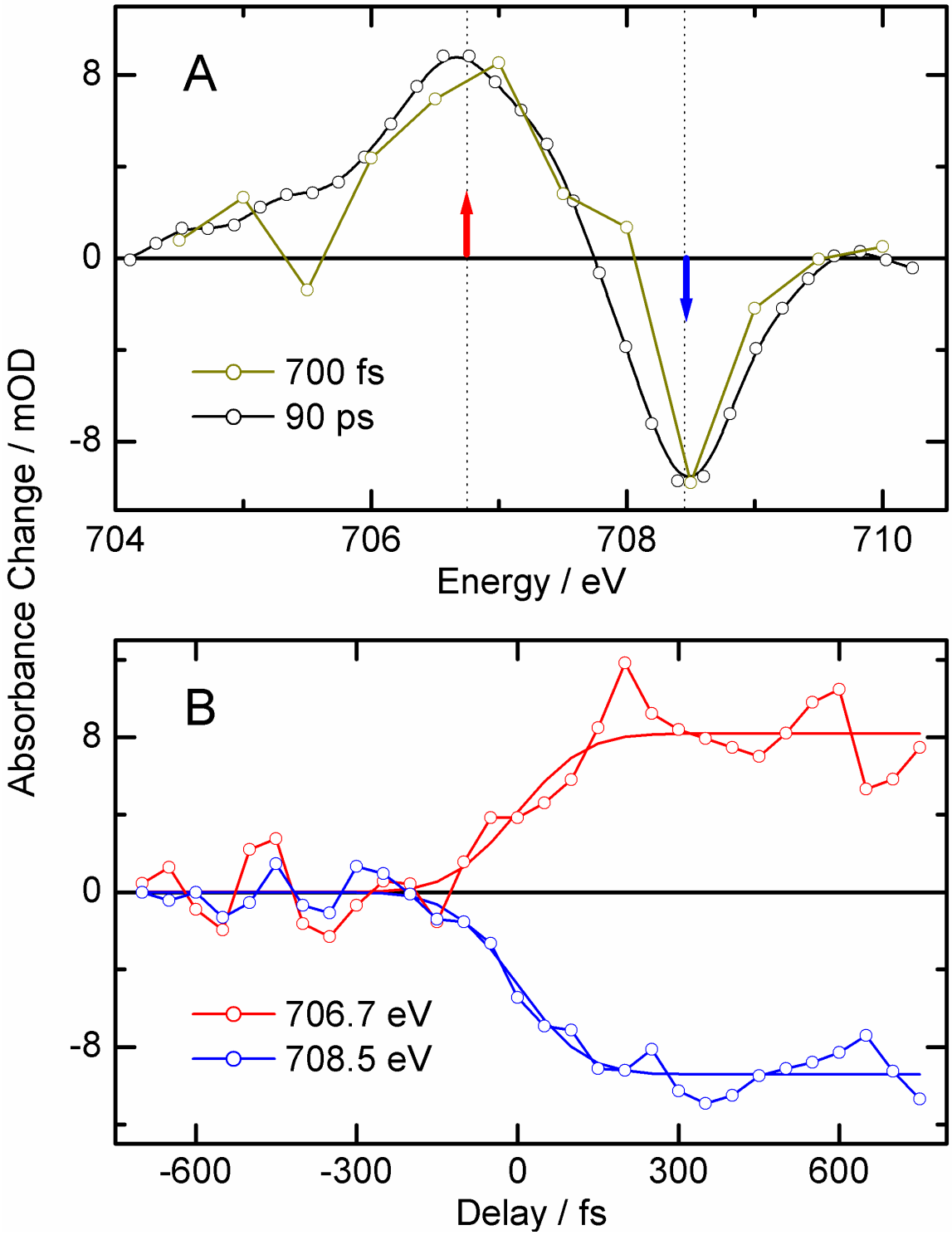
A
8
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700 fs
90 ps
704
706
708
710
Energy / eV
Absorbance Change / mOD
B
8
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-8
706.7 eV
708.5 eV
-600
-300
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Room-Temperature Ferromagnetic Mn-doped TiO2 Nanowires

강준하, 박정희, 손용재

고려대 소재화학과

Diluted magnetic semiconductors (DMSs), in which the host cations are randomly substituted by magnetic ions, have attracted a considerable amount of attention, because of their excellent potential as key materials for spintronic devices. The demonstration of the unique phenomena associated with DMSs, such as the field-effect control of their ferromagnetism, efficient spin injection to produce circularly polarized light, and spin-dependent resonant tunneling, has opened up a rich and various landscape for technological innovation in magnetoelectronics. Herein, Ti1-xMnxO ($0 \leq x \leq 0.03$) nanowires were synthesized by a combination of oxidation process of Ti foil and vapor transport of Mn. They consisted of single-crystalline nanocrystals, with uniform growth direction [110] or [110]. High-resolution X-ray diffraction showed no metal cluster formation. X-ray absorption spectroscopy and X-ray magnetic circular dichroism confirmed that the Mn2+ ions substitute into the coordinated sites. The magnetic moment measurement revealed room-temperature ferromagnetic behaviors. However, as the Mn content increases to 3 %, TiO2-Mn3O4 heterostructures are produced.

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Solvothermal synthesis of CdSe/ZnSe nanoparticles using ionic liquids as capping ligands.

송윤미, *장동명, *김한성, *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 approach the new aspects of ionic liquids in applications where the semiconductor nanoparticles (NPs) used as sensitizers of solar cells. Colloidal CdSe/ZnSe NPs were synthesized with a well-controlled shape and size through the novel use of the steric effect of the capping ligands. Trioctylphosphine oxide (TOPO) and octadecylamine (ODA) were used as coordinating co-ligands in the non-coordinating solvent, 1-octadecene (ODE). They can act as “sufficient” protection ligands, which can control the shape of the mono-dispersed NCs. The CdSe/ZnSe NCs were also synthesized using ionic liquids as co-ligand; C2MIM-TFSI, C4MIM-TFSI and P6,6,6,14-TFSI (anion=TFSI [(CF3SO2)2N-]). We studied the effects of ionic liquids on the yield and morphology of the NPs. Furthermore, we compared the optical properties, stablity and photocatalytic efficiency of the nanoparticles synthesized using both ODE and ionic liquids.

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Application of Nafion as a Membrane Separator in Membrane Introduction Time of Flight Mass Spectrometer

김현국, 김태규

부산대 화학과

Nafion is a commercially available perfluorosulphonate cation exchange membrane commonly used as a perm-selective separator in chlor-alkali electrolysers and as the electrolyte in solid polymer fuel cells. In this study, a Nafion membrane is used as the interface between the gaseous sample mixture and the vacuum in membrane introduction time-of-flight mass spectrometer. Temporal evolution of analyte through a 125-μm thick Nafion membrane was measured by monitoring the ion signal after a step change in the concentration of analyte. The results were explained by a non-steady permeation approximation. The diffusion coefficient, response time, selectivity, and detection limit were determined experimentally for a range of polar and nonpolar compounds. The results of the evaluation of Nafion membrane for membrane introduction mass spectrometry are discussed.

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Molecular Modeling Studies of Coprinus Cinereus Peroxidase (CiP) for High Stability in Severe Conditions

이주민, 장락우

광운대 화학과

Coprinus cinereus peroxidase (CiP) has been actively studied in recent years because of its applicability as the catalyst of radical polymerization reactions. But the unstability of CiP in severe conditions such as in organic solvents or at high temperature has limited its wide application. Hence, Molecular modeling studies have been performed along with a series of site mutation experiments to enhance the stability of CiP in these conditions.

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발표종류: 포스터, 발표일시: 목 15:00~17:00

Decoration of Silicon Nanowires Array with Gold and Silver Nanoparticles for High-Efficiency Surface-Enhanced Raman Scattering Substrates

백선영, 박정희, 조용재, 정경복

고려대 소재화학과

Surface-enhanced Raman spectroscopy (SERS) has attracted intense interest since 1977, because SERS has been extensively utilized to detect chemical and biological molecules. We introduce unique surface-enhanced Raman scattering (SERS) nanostructure substrates, which are made of a large-area arrays comprising silicon nanowires (Si NWs) decorated with gold nanoparticles (Au NPs) or silver nanoparticles (Ag NPs). The Si NWs arrays were produced through chemical etching of n-Si(100) wafer, and then deposited with the Ag NPs and Au NPs using various methods; (1) chemical bath deposition, (2) chemical bonding methods, (3) e-beam evaporation. The sizes were controlled in the range of 3-20 nm. Upon the excitation using a fs Ti-sapphire laser pulse (800 nm), the THz emission intensity exhibits strong enhancement for the NP deposition. The Raman scattering spectrum exhibits the same behavior as that of the THz emission. The results suggest that the deposition of noble metal NPs effectively enhances field enhancement by localized surface plasmons, which promise excellent new typed nanostructures for the SERS.

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Characterizing Amyloid-beta Protein Dimerization Process by Targeted Molecular Dynamics Simulations with Explicit Water

이제욱, 함시현

숙명여대 화학과

Ab42 peptide, the main cause of Alzheimer disease(AD), converts under some conditions from their non-toxic soluble structures into highly ordered toxic fibrillar agggregates. Because such transitions can provoke pathological conditions ranging from neurodegenerative disorder to systematic amyloidoses, much effort has been investigated in the development of various experimental and theoretical model systems to study the details of the aggregation process and the effects of endogeneous molecules that have been implicated in AD. In this study, all-atom targeted molecular dynamics (TMD) simulations in explicit water solvent were used to investigate the aggregation mechanism and dynamic properties of full-length aggregation-prone structures (APS) that founded from our previous conventional MD simulations. We mainly focus on the conformational changes of APS structures, formation (or deformation) of some important electrostatic interactions, and variations of hydrophobic properties. This study will contribute to improve understanding of progress and control the amyloid diseases.

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Estimations of Hydration Free Energies for Pyrophosphate in Aqueous Phase Using Three Dimensional Reference Interaction Site Model

이제욱, 이제욱, *Fumio Hirata, *Fumio Hirata, 함시현, 함시현

*숙명여대 화학과 *Institute for Molecular Science*

A recently developed statistical-mechanical theory of molecular solvation, especially the three-dimensional reference interaction site model (3D-RISM) theory, has an outstanding advantage in locating solvent molecules such as water and expectation for changes of hydration free energy in reactions. In this study, we present the hydration free energy calculation for the hydrolysis of pyrophosphates with several different charged states. The theoretical results herein will be compared with the experimental data. Also, we will discuss that the possible applications of 3D-RISM theory to debating problems in fields of biophysics and biochemistry.

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Fabrication of triad TiO_2 nano-bio composites: photoelectrochemical characterization

이형주, *Sreenivasan K.P., 윤민중

*충남대 화학과 *Nanyang University, Singapore*

TiO_2 nanomaterials have been widely studied as important substrate for solar cells. However due to its wide bandgap, it can only be activated by near-UV radiation, not by visible light which is dominant in the solar radiation. Thus, in this work nitrogen-doped TiO_2 nanochains coupled with silver ion (Ag+-N-TiO_2 nanochain) was formed, followed by adsorption with porphyrine(TTCP; Tetrakis(4-caboxyphenyl) porphyrine) and DNA(polyG-C·polyG-C, polyA-T·polyA-T) to fabricate the triad TiO_2 nanobio composites. It was found that the photoelectric conversion efficiency of the composite was highly improved depending on DNA base pairs.

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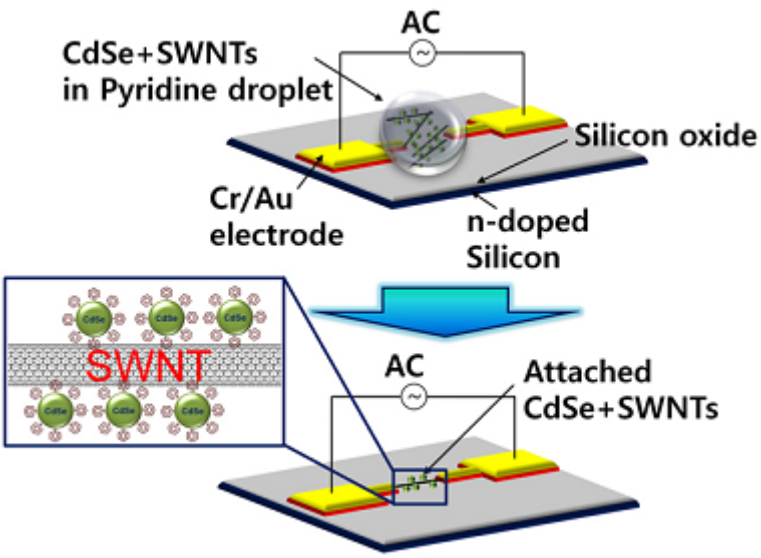
Efficient Electron Transfer in CdSe-py-SWNTs Hybrids : Optical and Elecrical characterizations

정소희, 한창수, 김경남

한국기계연구원 나노기계연구본부

Ability to transport extracted carriers from NQDs is essential for the development of most NQD based applications. Strategies to facilitate carrier transport while preserving NQDs' optical characteristics include: 1) Fabricating neat films of NQDs with modified surfaces either by adapting series of ligands with certain limitations or by applying physical processes such as heat annealing 2) Coupling of NQDs to one-dimensional nanostructures such as single walled carbon nanotubes (SWNTs) or various types of nanowires. NQD-nanowire hybrid nanostructures are expected to facilitate selective wavelength absorption, charge transfer to 1-D nanostructures, and efficient carrier transport.Even with the vast interests in using NQD-SWNT hybrid materials in optoelectric applications, still, no reports so far have clearly elucidated the optoelectric behavior when they were assembled on the FET mainly because the complexity involving in both components in their preparation and characterization. We have monitored the optical properties of both components (NQDs, SWNTs) from the synthesis, to the assembly, and to the device. More importantly, by using pyridine molecules as a linker to non-covalently attach NQDs to SWNTs, we were able to assemble NQDs on SWNTs with precise density control without harming their electronic structures. Furthermore, by measuring electrical signals from the fabricated aligned SWNTs-FET using dielectrophoresis (DEP), we were able to elucidate the charge transfer mechanism. S. Jeong et al., ACS Nano, 2010, 4 324-330



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Preparation of polyynes by laser ablation of graphite in various solvents

신승근, 박승민, 송재규, 하상수, 김일현

경희대 화학과

Laser ablation of graphite target in various solvents has been studied using a Nd:YAG laser(355, 532, and 1064 nm). Product analyses using UV and visble absorption spectroscopy. Linear hydrogen-capped polyynes($C_{2n}H_2$: n = 3, 4, 6) were formed in various solvents. We are able to confirm two kinds of polyyne's absorbance peaks in suitable experimental condition. Absorbance depends on laser power and ablation time.

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Highly Sensitive Immunoanalysis on a Hydrophilic/hydrophobic Hybrid Microarray Chip using Fluorescence and SERS Images Detection

이문권, 전향아, *이상엽, 주재범

*한양대 바이오나노공학과 *한양대 응용화학과*

Microarray-based protein chips and 96 well plate-based ELISA are most popular immunoassay techniques which have been used for the detection of target proteins. However, this method has some technical limits such as large sample consumption, coffee ring effect, poor limit of detection and low signal to noise ratio. In order to resolve these problems, we designed a conceptually new pre-patterened microarray chip for immunoanalysis. This chip was fabricated using MEMS (Micro Eelectro Mechanical Systems) processes. Here, pre-patterned hydrophilic spots are completely isolated from hydrophobic surfaces. In adddition, hydorophobic region is coated with Ti metal for the decrease of background signal. Then these hydrophilic spots were coated with amine monolayer or gold for a highly sensitive fluorescence and SERS (surface enhanced Raman scattering) detection. In this work, it is shown that the hydrophobic/hydrophilic hybrid property of the microarrays greatly improves the biomolecule deposition, spot uniformity, replication, and reproducibility. In this chip, less than 1 μL of reagent volume is required per each spot and any expensive spotter or arrayer is not needed for the sample immobilization. We used the fluorescence and SERS image based immunoassay techniques for the quantitative analysis of cancer markers detection by forming a self-assembled sandwich immunocomplexes immobilized on a pre-patterned microarray chip. In order to improve the sensitivity, alexa fluor dyes and hollow gold nanoparticles were used as highly sensitive probes for fluorescent emission and for Raman scattering, respectively. In this presentation, a sensitive immunoanalysis technique using this novel hydrophilic/hydrophobic hybrid microarray chip will be introduced.

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Preparation and Characterization of Single CrystallineNi-doped Ge Nanowires by Chemical Vapor Deposition

이우영, 김태규

부산대 화학과

Ni-doped Ge nanowires have synthesized via chemical vapor deposition (CVD) method. Homogeneous Ni-doped Ge nanowires are grown on a Au-coated Si substrate. The particle morphology and structure were characterized by scanning electron microscopy (SEM) and transmission electron microscopy (TEM). Ni-doped Ge nanowires are reacted for 20 min that resulted in high yield of homogeneous growth of diameter 60 ~ 120 nm and length up to several tens of microns. The Ni concentration (in at. %) as processed by energy dispersive x-ray (EDS) technique is about 5 %. The structure, optic and magnetic properties of Ni-doped Ge nanowires were investigated by X-ay diffraction (XRD) and photoluminescence (PL). The presence of Ni in Ge environment of chemical states is detected by X-ray photoelectron spectroscopy (XPS). We have compared Ni-doped Ge nanowires with undoped Ge nanowires for their different properties.

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Direct Fabrication of Single-walled Carbonnanotube Three-dimensional Networks as a Nano Filter for Micro-fluidic Devices

서정은, *이태재, 이해원, 김수환, 성명모

*한양대 화학과 *한양대 나노과학기술연구소*

Carbon nanotubes(CNTs) have been propised for use in pyriad applications, including elecronics, fuel cells, sensors, optical devices, and microfluidic applications. In this study, we report the fabrication of network of single-walled carbon nanotubes(SWCNTs) on Si pillar structure. Fe-Mo were used as the cocatalyst and deposited on substrate by a dipping method. CNT networks were grown by low pressure thermal chemical vapor deposition (CVD). These SWCNTs 3D network are used as nano filters for microfluidic device. 1 and 0.1 um PS nanopaticles were flew through microfluidic channel consisting SWCNT 3D networks. The results suggested that the SWCNTs networks should be coated with rigid materials to inhance thier structural strength by atomic layer deposition(ALD).

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Theoretical investigation of the reactivity in the C-F bond Activation of CH_3F by Os^+ in the gas phase

홍기룡, 김태규

부산대 화학과

The quartet and septet potential energy surfaces for the gas phase reaction between Os^+ and CH_3F were investigated using density functional theory. The molecular structures of intermediates and transition states were optimized at the B3LYP level for both C-F and C-H bonds activation pathways. All transition states were identified by using the intrinsic reaction coordinate method. According to the revealed mechanisms and the calculated potential energy surfaces, HF-elimination is the most favorable product channel which has a smallest barrier height. The results of this study were compared with the experimental observations.

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Fabrication of Nano-Structured ZnPc Thin Films by Facile Solvent Vapor Treatment

김진현, *공혜진, 임상규

*국민대 생명나노화학과 *국민대 화학과*

Over the past decade, organic semiconductors are attracting growing attention for their potential in a wide range of optoelectronic device applications. Thin film morphology is known to play a crucial role in the performance of these devices. In particular, the controlled nano-structure with a high contact area between the electron-donating and accepting layers is necessary to improve the energy conversion efficiency of organic photovoltaics. Previously reported research works to fabricate such a well-organized nano-structures such as nano-imprinting, surface-directed demixing template and a nematic gel template, however, are not so effective and very complicated. In this study, we suggest a solvent vapor treating method which provides relatively simple and effective way to control the nano-structured surface of zinc phthalocyanine (ZnPc) thin films. The films were deposited by organic molecular beam deposition (OMBD) and the surface morphology was observed using atomic force microscopy (AFM) and field emission scanning electron microscopy (FE-SEM).

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Morphology Evolution and Growth Behavior of SubPc Thin Films

류일환, *허일수, 박찬량, 곽현태, *임상규

*국민대 화학과 *국민대 생명나노화학과*

The surface structure, morphology and growth behavior of Chloro[subphthalocyaninato]boron(Ⅲ) (SubPc) thin films deposited by organic molecular beam deposition(OMBD) have been studied using atomic force microscopy (AFM), x-ray diffraction (XRD) and height difference correlation function (HDCF) analysis. The evolution of surface morphology for SubPc thin films is significantly different from other regular phthalocyanines. Elongated and branched, so-called ramiform, clusters are formed at the initial stage of the film growth. Surface roughness of the films increases at first and then decrease after the empty space between the cluster starts to be filled. The crystallinity and spectroscopic properties of the films with various thicknesses as deposited and annealed are also investigated.

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Tertiary and quaternary Conformational Change in Homodimeric Hemoglobin revealed by Time resolved wide angle scattering

muniyappan srinivasan, *왕기영, 이효철

*KAIST 화학과 *KAIST 나노과학기술대학원*

Allosteric structural transition of hemoglobin upon ligand binding is an important mechanism yet to be understood completely. The allosteric process is closely associated with cooperative ligand binding and ligand induced structural changes. These structural changes are directly related to the function and reactivity of the protein. Allosteric transition in Human hemoglobin is coupled with tertiary and quaternary structural changes, in addition the structural propagation between allosteric sites are complex due to heteromeric nature. In this regard, HbI is a suitable model system to study the allosteric mechanism due to its simple homodimeric nature. The R-T transition in HbI constitutes mainly of tertiary structural changes like flipping of the Phe97 from subunit interface towards the proximal heme pocket, reorganization of an interfacial water cluster, movement of the heme group toward the subunit interface and a small subunit rotation of 3.3°. Here, we have investigated the ligand dissociation and allosteric structural transition of HbI by Time resolved wide angle scattering.

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Mapping the Conformational changes in myoglobin on CO photodissociation using Time-resolved solution X-ray scattering

김영민, 김종구, *왕기영, **이재혁, **이효철

*KAIST 화학과 *KAIST 나노과학기술대학원 **KAIST 화학과*

Here we report the tracking of the transient helix motions of myoglobin in response to the ligand photodissociation of carbonmonoxy myoglobin (MbCO) within the timescale 100 picoseconds (ps) to 10 milliseconds (ms). Analysis of Time-resolved X-ray solution scattering data of myoglobin was performed to reveal the dynamics of protein helical motion after CO photodissociation using rigid body molecular dynamics simulation. On photodissociation, A, B, E, H helix moves closer to heme and C, D, F helix moves away from the heme at 100ps. And within 1n the A, F, G, H helices are observed closer towards the heme and the B, C, D helices move away from the heme. The results of our data analysis indicate that displacement of the B, F helix toward the heme occurs within 100ps and that reverse movement of the helices takes place suggesting B, F helices breathing motion with a time constant of a few hundred ps. This observations are consistent with the previous results reported by time resolved UV-Resonance Raman Spectroscopy. Hence we suggest a mechanism in which protein tertiary structural changes are propagated after photodissociation from the heme through helix by observing the breathing motion of helices. And the results strongly suggest the capability of combining TR-WAXS data and rigid body molecular dynamics simulation in detecting the conformational change of proteins in solution.

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Density Functional Theory study of the catalytic mechanism and activity of Cu phenanthroline and its substituted derivative on O2 reduction reaction

chenjunxian, 김찬경, 김창곤, 이해황, 한인숙

인하대 화학과

In this study, density functional theory is used to study the catalytic mechanism of Cu phenanthroline complexes and catalytic activity of its substituted derivatives. By examining adiabatic electron affinities and structure of end-on and side-on binding modes with O2 and H2O2 , the four electrons mechanism, partly with company of two electrons mechanism for H2O2 intermediate are obtained. Electronic properties, such as ionization and Muliken charge are evaluated to investigate the Substitution effect of the catalyzer. All the results are compared with the experiment of finding.

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Morphology and photoconductivity of poly-N-vinylcarbazole-cellulose triacetate Langmuir-Schaefer films

조은애, 허도성, C. Basavaraja

인제대 화학과

Cellulose triacetate (CTA) was doped with poly(N-vinylcarbazole) (PVK) via the oxidative polymerization of N-vinylcarbazole with ferric chloride to form polymer blends. Langmuir-Schaefer (LS) films of the polymer blends were fabricated. The morphology of the cellulose triacetate-poly(N-vinylcarbazole) (PC) blends were analyzed using transmission electron microscopy (TEM). The pressure–area isotherm of PC blends revealed the possibility of compact monolayer formation at air–water interface. The voltammetric investigation of PC blends showed an appreciable electrochemical behavior. The photoinduced charge transfer across a donor/acceptor hybrid interface provided an effective method to study the photoelectrochemical properties of the PC polymer films.

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Thermal conductivity in cellulose triacetate-Multiwalled carbon nanotube polymer films

C. Basavaraja, 허도성, 조은애, 김봉성

인제대 화학과

The present work describes the preparation and the study of thermally stimulated discharge conductivity (TSDC) study of Cellulose triacetate (CTA) – multiwalled carbon nanotubes (MWNTs) film thermoelectrets. TSDC has been carried out in the temperature range 308–503 K and at four different polarizing fields. The conductivity of the polymer blends increased with increases in temperature showing a semi-conducting behavior. The apparent activation energy also showed a pronounced effect with the increase in the content of MWNTs.

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Effect of amphiphilic copolymer containing $Ru(bpy)_{32+}$ on the formation of honeycomb pattern

김봉성, 허도성, C. Basavaraja, 조은애

인제대 화학과

A new functional amphiphilic polymer (AP) containing photo-catalytic Ru(bpy)32+ was synthesized and honeycomb patterns were obtained by casting polymer solution of polystyrene and different concentration of AP under humid condition. The copolymer was obtained by the radical copolymerization of ruthenium(4-vinyl-4'-methyl-2,2'-bipyridine)bis(2,2'-bipyridine)bis(hexaflurophosphate) with N-dodecylacrylamide and N-isopropylacrylamide. The results demonstrate that high porous regular patterns are greatly affected by added concentration of AP, pore size of the pattern and the height of the hole grow larger with the increase of AP polymer ratio. However, further increase in AP polymer causes the irregularity of the patterns and mixed patterns with small size also are occurred by the effect of strong hydrophilicity induced by the ion charge of the ruthenium ion.

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High-level expression and purification of the second transmembrane domain of wild-type and mutant human melanocortin-4 receptor for solid-state NMR structural studies

박태준, 강가애, 김용애

한국외국어대 화학과

It has been demonstrated that human melanocortin-4 receptor (hMC4R) plays an important role in the control of energy homeostasis, and heterozygous mutations in the hMC4R gene are the most frequent genetic cause of severe human obesity. In order to obtain additional insight into the structure and function, we cloned, expressed, and purified the second transmembrane domain of the wild-type hMC4R (wt-TM2) and D90N mutant hMC4R (m-TM2). To facilitate structural studies of these hMC4R by solid-state NMR, efficient methods for the production of milligram quantities of isotopically labeled protein are necessary. However, large-scale production of most transmembrane proteins has been limited by experimental adversities due to insufficient yields and low solubility of protein. Nevertheless, through the optimization of the expression and purification approach, we could obtain uniformly or selectively labeled fusion proteins in yields as high as 200–250 mg per liter M9 minimal medium. These proteins were overexpressed in inclusion bodies as a fusion protein with ketosteroid isomerase (KSI) in Escherichia coli, and the fusion protein was purified using immobilized metal affinity chromatography under denaturing conditions. wt-/m-TM2 peptides were released from the fusion by cyanogen bromide cleavage at the Met residue and separated from the carrier KSI by size exclusion chromatography. Initial structural data obtained by solution and solid-state NMR measurements of wt-/m-TM2 is also presented. The successful application to the production of the second transmembrane domain of human MC4R indicates that the method can be applied to other transmembrane proteins as well and also enable its structural and functional studies using solid-state NMR spectroscopy.

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Structural and optical characteristics of CuO thin films

김재욱, 차병관, 지명진, 박병천, 경동현, 김종규

단국대 화학과

We synthesized copper oxide (CuO) nano particles. Copper oxide thin films were deposited onto glass substrates by spin-coating method, from a precursor solution contaning copper acetate, ethanol and ammonium hydroxide. After deposition, the films were heated at a temperature of 100℃ in order to remove unwanted materials. Finally, the films were annealed at 500℃ for complete oxidation. The formation of copper oxide has been confirmed by x-ray powder diffraction (XRD), scanning electron microscopy (SEM), UV/Visible spectrometer (UV) and photoluminescence spectrometer (PL). The crystallites are preferentially oriented with (0 0 2) planes parallel to the substrate surface. The analysis UV/Visible spectra shows the direct nature of band-toband transitions. The optical bandgap energy of 1.2eV.

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Solvothermal synthesis of ZnO nanorods in different alcohols

김재욱, 차병관, 지명진, 권태필, 경동현, 김종규

단국대 화학과

Solvothermal reaction of zinc acetate in various alcohols. The fomation of zinc oxide (ZnO) nano rods. The formation of copper oxide has been confirmed by x-ray powder diffraction (XRD), scanning electron microscopy (SEM), and infrared (IR). It was found that average diameter and length of the nano rods increased with an increase in reaction temperature or the initial concentration of zinc acetate. On the contrary, the aspect ratio of the product depended upon type of alcohol used as the reaction medium. An investigation of the reaction mechanism suggested that the formation of ZnO nano rods was initiated from the esterification reaction between zinc acetate precursor and alcohol to from ZnO seeds.

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Synthesis of nanocrystalline CuO powder via sol–gel method.

차병관, 김재욱, 지명진, 권태필, 박병천, 김종규

단국대 화학과

This reports the growth mechanism of sol-gel derived nanocrystalline CuO powder. The influence of pH value of the sol on the crystallite size, morphology and structure of CuO powder was investigated by using X-ray diffraction, scanning electron microscopy. The growth mechanism of CuO particles from Copper acetate hydrate precursor by the sol–gel process has been discussed in terms of solvation, hydrolysis and polymerization. The synthesized CuO powders were successfully used as the electrode material for dye-sensitized solar cells.

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Expression and Purification of Transmembrane Domain of Syndecan-4 for Solid-state NMR Structural Studies

박태준, 이민혜, 김용애

한국외국어대 화학과

Syndecan-4 is a transmembrane heparan sulfate proteoglycan belonging to the syndecan family and they are present on most cell types. Syndecan-4 is known to bind to various molecules, such as basic fibroblast growth factor, midkine, and tissue factor pathway, via its heparan sulfate chain, and is thought to play many biological roles through its binding bio-mediators. To get better understand the mechanism and function of Syndecan-4, it is critical to elucidate the three-dimensional structure of it. Unfortunately, determination of structure of Syndecan-4 is very difficult because it is membrane-bound protein that transverse the lipid bilayer of the cell membrane, so large-scale production of such integral membrane proteins has been limited by experimental adversities due to insufficient yields and low solubility of protein. And also it is hard to characterize the membrane-bound three-dimensional structure using conventional solution NMR and X-ray crystallography.Here, we have been optimized the large scale expression conditions and the purification system to get the target membrane protein to high purity. Purification of the peptide was carried out by reversed-phase HPLC. And the purified product was checked by a NMR studies in solution. We will also research the solid-state NMR structural studies of Syndecan-4 transmembrane protein.

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Novel Chemical Kinetics for a Single Enzyme Reaction:Relationship between Substrate Concentration and the SecondMoment of Enzyme Reaction Time

박보정

중앙대 화학과

We report a robust quadratic relation between inverse substrate concentration and thesecond moment, $< t^2 >$, of a catalytic turnover time of a single enzyme reaction. The resultholds irrespective of the mechanism and dynamics of the enzyme reaction, and suggests anovel single molecule experimental analysis that provides information about reactionprocesses of the enzyme-substrate complex and ergodicity of the enzyme reaction system,which is beyond the reach of the conventional analysis for the mean reaction time, $< t >$. Itturns out that $< t^2 > -2 < t >^2$ is linear in inverse substrate concentration for a homogeneousergodic enzyme system, and its value at the high substrate concentration limit provides directinformation about if any non-Poisson reaction process of the enzyme-substrate complex. Fora non-ergodic heterogeneous reaction system, the corresponding quantity becomes aquadratic function of inverse substrate concentration. This leads us to suggest an ergodicitymeasure for single enzyme reaction systems. In obtaining the results, we introduce a novelchemical kinetics applicable to a non-Poisson reaction network with arbitrary connectivity, asa generalization of the conventional chemical kinetics.

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investigation of the phase transition of poly vinylidene fluoride

허원준, 양혁, 이억균

KAIST 화학과

The phase transition of poly-vinylidene fluoride(PVDF) from α-phase to β-phase is investigated using molecular dynamics simulation and DFT calculation. The phase of PVDF is the most important factor determining the dielectric and ferroelectric properties of PVDF. We trace the energy change during the phase deformation and suggest the phase change mechanism. From the potential energy surface calculated by computer simulation, the transition pathway is analyzed. The energy barrier between termodynamically stable α-phase and β-phase can be overcome by impressing electric field to the PVDF film.

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A Molecular Simulation Study of Structural and Dynamic Properties of Mixed DPPC/DPPS Bilayers

정현태, 성봉준

서강대 화학과

Cell membranes have been studied extensively since they play critical roles in many physiological processes. After it has been realized that cell membranes consist of various kinds of molecules such as lipids, proteins, cholesterols, and bound ions, the effects of their compositions on the dynamics and the structure have been of great interest. For example, ions bound to the cell membranes may determine the electrostatic fields near the cell membranes; thus further influencing physiological processes such as the peptides penetration through the membrane. Such an effect of the bound ions may be tuned as one changes the compositions of cell membranes. In this work, we employ molecular dynamics simulations to investigate the microscopic details of the interactions between lipid bilayers and ions. We change the compositions of the lipid bilayers by mixing DPPS (negatively charged) lipids and DPPC (neutral) lipids. We study the structure and the dynamics of lipid bilayers of different compositions using Voronoi tessellations. It is found that the order parameter of the alkyl chains, the dynamics of surface areas of lipids and the surface area distributions are sensitive to the compositions of lipid bilayers.

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Mesophase Transition of Porous Silica with Controlled Templating Method of PS-block-PEO Copolymer

김창우, 문봉진, 강영수

서강대 화학과

We examined the mesophase transition from disorder to the lamellar for the porous silica using diblock copolymer, polystyrene-b-polyethylene from transmission electron microscopy and small-angled X-ray scattering. The geometrical structure is monitored during the phase-transformation of mesoporous silica synthesized through evaporation-induced self assembly. The phase ordering phase depend on the concentration of polymer and the polystyrene block in the cores of organic-inorganic composite. Mechanisms of formation of the silica meso-structures are proposed and should be very much useful for the understanding of the phase transition of meso structured materials.

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발표종류: 포스터, 발표일시: 목 15:00~17:00

Preparation of conducting silver paste with Ag nanoparticles prepared e-beam irradiation

손종화, *강영수

*서강대 화학과 나노구조물연구실 *서강대 화학과*

Conducting silver pastes were prepared by using Ag nanoparticles prepared with e-beam irradiation (from KAERI) and its conductivity was comparatively studied with Ag nanoparticles prepared by thermolysis method (commercial). Among the conductivities of various weight% of silver nanoparticle in the conducting silver pastes, silver paste with 90 wt% of silver nanoparticle has the highest conductivity as 1.6×10^4 S•cm^{-1} of conductivity. This conductivity value is 1.6 times higher than the Ag pastes prepared by thermolysis method and has been commonly used in commercial way. The e-beam irradiated silver nanoparticle which has ~150 nm size is mixed with glass frit and is sintered for 1 hour in 500 °C. This is interpreted as the narrow size distribution and homogenous dispersion of Ag nanoparticles in the pastes.

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Conversion of Blue-Red Emission to Pure Blue Emission for $CaMgSi_2O_6:Eu^{2+}$

Amor Uttaam Pawar, Abhijit Pandurang Jadhav, 강영수

서강대 화학과

Nanoparticles of $CaMgSi_2O_6:Eu^{2+}$ were synthesized by co-precipitation method using ethanol as a solvent. Calcinating these nanoparticles at 1100 ^oC in ambient atmosphere for 2 hrs, dual emission blue (450 nm) as well as red (615 nm) emission with dual excitation wavelength 337 and 395 nm, was observed respectively. When the calcination was carried out in presence of N_2-H_2 (96-4%) at 1100 ^oC for 2 hrs, only blue emission was observed with 337 nm excitation wavelength. Reduction of Eu^{3+} was carried out in presence of N_2-H_2 to Eu^{2+} which was responsible for blue emission with 84% increase in luminescence intensity.

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Wavelength Converting Nanocomposite Films Using Red and Blue Phosphor for Greenhouse Effect

Abhijit Pandurang Jadhav, Amor Uttaam Pawar, 강영수

서강대 화학과

The solar energy passing through the atmosphere is responsible for number of phenomenon. A portion of the energy is reflected back to space and some part of energy is absorbed by atmospheric gases like ozone. Most of the energy passing through the earth's atmosphere is utilized by plants for photosynthesis and for heating the earth's surface. The ultraviolet portion of the sunlight reaching the earth's surface is less intense than other portions of the spectrum. The environment where UV light is blocked is not suitable for harmful insects like aphids, cockroaches and vermins which are phototaxis to the ultraviolet light. Thus conversion of the UV portion of the solar spectrum into visible and near IR is essential for better utilization of energy as well as insect control. The nanocomposite films prepared by blow extrusion technique using red ($Y_2O_3:Eu^{3+}$; 3.3 wt%) and blue ($CaMgSi_2O_6:Eu^{2+}$; 4.2 wt%) phosphors with LDPE and EVA polymers shows better wavelength converting properties with high transmission to visible light.

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The role of impurity atoms in bcc/fcc iron system

양혁

KAIST 화학과

The electronic and mechanical properties of metallic iron have been of interest for many years. It is well known that grain boundary site acts as crucial factor for mechanical stability of metallic structure. Impurity atoms in the grain boundary can strengthen or embrittle the metal system. Boron has an extremely good record in improving intergranular cohesion in metals while phosphine cause impurity embrittlement. Bulk iron contains many other elements. Some of them stabilize and strengthen iron system and some of them don't. We employ a first principles method based on the density functional theory (DFT) with the generalized gradient approximation (GGA) to analyze impurity atoms in iron system with grain boundary. We calculated grain boundary structures in both of bcc and fcc structure. The impurity atoms are located in substitutional site, tetrahedral interstitial site, or octahedral interstitial site. We consider the impurity atom site according to the atom size and the space in iron lattice structure.

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Excess Grand Potential for a System under an External Field: Effects of External FieldDriven Nonextensivity

임유림, 성재영

중앙대 화학과

We report that an external field can drive inherently extensive systems into nonextensive ones. For the correct grand canonical description of nonextensive systems, it is necessary to take into account the excess grand potential, X, in addition to the conventional grand potential proportional to the thermodynamic pressure, which has long been overlooked in the literature in this field. We present the statistical mechanical expression for X of a system as a functional of the external field imposed on the system, from which we establish the criterion for the external field that drives an inherently extensive macroscopic system into a nonextensive one.

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Epitaxially driven FeSi nanowire growth from supported FeSi seed structure

김시인, *윤하나, *김봉수

*KAIST 나노과학기술대학원 *KAIST 화학과*

Directionally-grown single-crystalline FeSi nanowires (NWs) have been successfully synthesized on a m-plane sapphire substrate by chemical vapor transport method without catalyst. X-ray diffraction and transmission electron microscopy revealed that the NW has a simple cubic B20 crystal structure. We observed seed crystals with various shapes along together with FeSi NWs on the substrate. We show that the directionally-grown NWs grow from the seed crystals by a correlation the geometry and growth orientation of the seed crystals with those of NWs. In addition, it is possible to control the diameter of as-synthesized FeSi NWs by changing the ratio of silicon powder on graphite powder in the mixture as the silicon source. Synthesis of aligned NWs on a substrate in selected orientation is highly valuable to fabricate three-dimensional (3D) integrated platform. Therefore, the directionally grown FeSi NWs could be employed for development of advanced 3D nanodevices.

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Synthesis of Half-metallic Fe3Si Nanowires

김시인, *인준호, *윤하나, *김봉수

*KAIST 나노과학기술대학원 *KAIST 화학과*

We report diffusion-driven crystal structure transformation method to fabricate half-metallic Fe_3Si nanowires (NWs) from paramagnetic FeSi NWs. Fe_3Si is a representative half-metallic material, showing high Curie temperature of 840 K and superb spin polarization. Fe_3Si NW, however, has not been synthesized yet in spite of many successful synthesis of various magnetic silicide NWs. FeSi is converted to Fe_3Si by high temperature thermal annealing in diluted O_2 condition. Transmission electron microscopy (TEM) studies show distinct change of the NW morphology and diameter and indicate that the NW after SiO_2 shell-etching is single-crystalline Fe_3Si with fcc crystal structure. Magnetic properties of the Fe_3Si NWs have been studied using a superconducting quantum interference device (SQUID) magnetometer. As-synthesized Fe_3Si NWs show high-temperature ferromagnetic properties with a Curie temperature of much higher than 370 K. The half-metallic Fe_3Si NWs can be employed as an important building block in the development of spintronic devices. Our newly-developed NW crystal transformation method would be valuable as a general method to fabricate metal-enriched silicide NWs that are difficult to synthesize otherwise.

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Conformational Change of DNA-DNA Polymerase Complex Induced by Artificial Nucleotide Derivatives

임영빈, *김성근

*서울대 생물물리 및 화학생물 *서울대 화학부 & 서울대 생물물리 및 화학생물학과*

DNA polymerase (DNAP) copies a DNA template sequence and transfers the genetic information, which is the crucial activity for the development and maintenance of organisms. Here we report that artificial nucleotide derivatives, such as peptide nucleic acid, locked nucleic acid, and dideoxyribonucleic acid, induce conformational change in DNA-DNAP complex when DNAP binds to a modified DNA template during replication. Since the sugar backbone of nucleic acids closely interacts with the enzymatic active site of DNAP, we anticipate that modification of sugar backbone would affect the conformational change of DNAP. Using single-molecule fluorescence resonance energy transfer, we investigated the effect of sugar backbone on the conformational change of DNA-DNAP complex.

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Synthesis and Characterization of Hexagonal FeGe Nanowires

윤하나, 김봉수

KAIST 화학과

We report the synthesis of single-crystalline freestanding hexagonal FeGe nanowires for the first time. The nanowires are grown on a sapphire substrate using a simple vapor transport synthetic process without any catalyst. As-grown FeGe nanowires are ferromagnets, with the Curie temperature above room temperature, higher than that of bulk hexagonal FeGe. In addition, the FeGe NWs have grown on a conducting HOPG substrate. Field emission properties of the NW arrays are investigated and the NW arrays have exhibited efficient field emission properties compared to previously reported other emitters such as metal silicide NWs.

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Single-Crystalline Ferromagnetic Ni3Co Nanowires

윤하나, 김봉수, 인준호

KAIST 화학과

We report synthesis of vertical Ni3Co nanowires on a c-plane sapphire substrate by chemical vapor transport method. A vapor-solid-solid mechanism was proposed for Ni3Co nanowire growth, which was catalyzed by Ni3Co2 nanoparticle at the tip. As-synthesized vertically aligned single-crystalline Ni3Co nanowires exhibit strongly ferromagnetic properties. Such single-crystalline ferromagnetic alloy nanowires could be important in the application of spintronics such as nonvolatile memory devices. We could also control the composition of the nanowire by adjusting experimental conditions, producing Ni, Ni3Co, and NiCo nanowires.

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Effect of acidity and water concentration on the synthesis of porous chromium-benzenedicarboxylates

전종원, 정성화

경북대 화학과

In the present work, two metal-organic frameworks (MOFs), Cr-benzenedicarboxylates such as MIL-53 and MIL-101 have been synthesized in a wide range of reaction conditions in order to understand the effects of water concentration and acidity. It is found that MIL-101 is preferentially obtained when the water content is high and acidity is low. On the contrary, concentrated reactants and high acidity lead to the formation of MIL-53. The steady conversion of MIL-101 into MIL-53, due to difference in relative stability, with the progress of reaction is also confirmed. The effect of water, therefore, may be explained by the increase of synthesis rate with increasing concentration of reactants. The MIL-53 is selectively obtained at low water content because the MIL-101, a transient phase, even if it is formed initially, may be converted into MIL-53 due to a high reaction rate. Relatively low acidity (high pH of about 3) is beneficial to the synthesis of MIL-101 even though increased MIL-53 yield was expected at low acidity due to the accelerated deprotonation of terephthalic acid. The selective formation of MIL-101 at low acidity is probably because the concentration of a chromium trimer (the chromium species that are essential for the MIL-101 structure) increases with increasing pH. The concentration of Cr trimer is more important than the concentration of benzenedicarboxylate for the synthesis of MIL-101.

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A kinetic study on the synthesis of a metal-organic framework material, iron-terephthalate under ultrasound, microwave and conventional electric heating

Enamul Haque, Nazmul Abedin Khan, 정성화

경북대 화학과

A metal-organic framework material, iron-terephthalate, has been synthesized sovothermally at relatively low temperature with not only conventional electric (CE) heating but also irradiation under ultrasound (US) and microwave (MW) to understand the accelerated syntheses by US and MW. The kinetics for nucleation and crystal growth has been analyzed by measuring the crystallinity of the Fe-BDC at various conditions. The nucleation and crystal growth rates have been estimated using crystallization curves representing the change of crystallinity with the reaction time. The activation energy and pre-exponential factor have been calculated from the Arrhenius plot. It has been confirmed that the rate for crystallization (both nucleation and crystal growth) is in the order of US > MW >> CE, and the accelerated syntheses under US and MW are due to increased pre-exponential factor rather than decreased activation energy. It is suggested that physical effect such as hot spots is more important than chemical effect in the accelerated syntheses with US and MW. The syntheses have also been conducted in two steps to understand quantitatively the acceleration by MW, and it has been found that the acceleration in crystal growth is more important than that in nucleation even though both processes are accelerated by MW.

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Effect of metal ions on the kinetics of synthesis of isostructural porous metal-benzenedicarboxylates

Enamul Haque, 정성화

경북대 화학과

A few porous isostructural metal-benzenedicarboxylates (Me-BDCs) such as MIL-47(V), MIL-53(Al) and MIL-53(Cr) have been synthesized hydrothermally from metal chlorides, TPA (terephthalic acid) and water to elucidate the relative rates (both in the nucleation stage and crystal growth stage) depending on the metal ions. The synthesis rates are r MIL-47(V) > r MIL-53(Al) > r MIL-53(Cr) for both in the nucleation and crystal growth stages at the same temperature, illustrating the importance of lability of the metal ions in the synthesis rate of a MOF material. The lability of metal ions is important in the kinetics of MOF synthesis because the synthesis may be carried out by simple complexation or ligand exchange. The importance of the lability of metal ions may suggest that the deprotonation rate of TPA (to BDC), even in an acidic condition, is relatively fast compared with the complexation rate of BDC on metal ions to form MOFs.

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Phase-selective synthesis and phase-transition of porous chromium-benzenedicarboxylates

Nazmul Abedin Khan, 정성화

경북대 화학과

A study of the crystallization of two topical porous chromium- benzenedicarboxylates, denoted as MIL-53 and MIL-101, has been reported. Both conventional electric (CE) and microwave (MW) heating have been explored in order to understand phase-selectivity and phase-transition between these solids. One chromium benzenedicarboxylate, the kinetically favorable MIL-101 (lower density phase) is the phase obtained at the early stage of the reaction while thermodynamically favorable MIL-53 phase (higher density phase) is obtained at the expense of MIL-101 at longer synthesis time. Phase-transition from MIL-101 to MIL-53 does not occur by direct conversion. Instead, at the longer synthesis time the MIL-101 is degraded, and subsequently, MIL-53 is observed via the reorganization of the decomposed species. Moreover, it is suggested that MW irradiation provides a phase-selective synthesis of MIL-101 due to rapid synthesis, preventing the conversion into the thermodynamically favorable phase (MIL-53). Therefore, the MW synthesis may lead to a new way to find new metal-organic frameworks (MOFs) especially that is hard to synthesize due to interconversion into a more stable phase or dense phase.

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Purification of porous metal terephthalates with ultrasonic treatment in the presence of amides

강인중, Enamul Haque, Nazmul Abedin Khan, 정성화

경북대 화학과

A facile purification method of metal-organic frameworks (MOFs), especially the ones containing insoluble 1,4-benzenedicarboxylic acid (terephthalic acid) in the pore, has been suggested. The purification method is composed of treating the MOF with amides such as N, N-dimethylformide, especially under ultrasound. The purification is completed in 1 h at 70 oC as has been confirmed by XRD, nitrogen adsorption, FTIR and TGA, etc. The purification method is simple, one-step, fast and energy-efficient. The MOFs purified by the proposed method show high surface area and micropore volume, showing the efficiency of the method. The suggested purification method will lead to a new way to activate (for example, to remove carboxylic acids) MOFs that are especially unstable above around 100 oC. Additionally, the method may be used to transform a non-porous MOF-type material into a porous MOF structure. However, adequate solvents will be necessary for the facile purification of MOFs.

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Anionic Charge Division in Dibromobenzene

손태일, 김남두, 이상학, *김성근

*서울대 화학부 *서울대 화학부 & 서울대 생물물리 및 화학생물학과*

We investigated the anion of 1-,(2, 3, or 4)-dibromobenzene (DBB) using anion mass spectrometry, photoelectron spectroscopy, and theoretical calculations. The monomer anion of all three DBB species was clearly detected by mass spectrometry, indicating that their electron affinities are positive. Photoelectron spectroscopy revealed that the electron affinity of these species is strongly dependent on the relative position of the Br atoms, in contrast to the case of bromochlorobenzene. We found that a dissociative state of neutral DBB is associated with the photodetachment of electron from anionic DBB. We also investigated the molecular orbitals of DBB species by density functional theory calculations and found that the excess electronic charge of the anion is equally divided at the local site of the Br atoms, whose parallel in the case of cation has recently been reported.

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Patterned Multiplex Pathogen DNA Detection by Au Particle-on-Wire SERS Sensor

강태준, 김봉수

KAIST 화학과

An Au particle-on-wire system that can be used as a specific, sensitive, and multiplex DNA sensor is developed. A pattern formed by multiple Au nanowire sensors provides positional address and identification for each sensor. By using this system, multiplex sensing of target DNAs was possible in a quantitative manner with a detection limit of 10 pM. Target DNAs from reference bacteria and clinical isolates were successfully identified by this sensor system, enabling diagnostics for infectious diseases.

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Ultrasensitive Single Nanowire on a Film SERS Sensor for Hg2+ Detection

강태준, *이상엽, **주재범, 김봉수

*KAIST 화학과 *한양대 응용화학과 **한양대 바이오나노공학과*

We report a single nanowire on a film (SNOF) SERS sensor for Hg2+ detection based on a structure-switching aptamer. This sensor provides reproducible SERS signals only in the presence of Hg2+ with a low detection limit of 100 pM. Moreover, high selectivity, stability, and reusability of this sensor are achieved.

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Plasmonic Properties of Single Nanowire on a Film

강태준, 안지희, 김봉수

KAIST 화학과

Single Nanowire on a Film (SNOF) structure is a well-know surface-enhanced Raman scattering active platform. We demonstrated the polarization dependent SERS signals of SNOF and investigated the surface plasmon propagation of this structure. The localized surface plasmon resonance spectra were also measured by the side-illumination methods.

대한화학회 THE KOREAN CHEMICAL SOCIETY

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Proton transferfing systems on Ice Ih surface ; Comparative Study

배태열, 최철호

경북대 화학과

Ice Ih(hexagonal ice) is general form of ice type with Ice Ic(cubic ice). Especially study for protonation which occur on the surface, barrier and transition state form of transferring proton one H_2O to other H_2O on ice surface didn't reported except inside transfer system. B3LYP correlation functionals, 6-31G** basis set and reproduce for original ice system we use freezing of atom from original coordiantes.

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Highly efficient NTSC blue OLED with the novel pyrene molecule acting as both an emitter and an electron transporter

오형윤, *이성훈

*서울대 화학부, LG Display R&D center *서울대 화학부*

The maximum external quantum efficiency of 4.8 % at 1931 CIE color coordinate (x, y) of (0.147, 0.081) is achieved at 1000 cd m-2 from simply synthesized 1,6-bis(N-phenyl-2-pyridylamino)pyrene (PPyP) which functions as both an emitter and an electron transporter in an OLED. The PPyP compound shows, as an emitter, a saturated deep blue photoluminescence (PL) spectrum coincided with 1931 CIE (0.147, 0.071) with high quantum yield in CHCl3 solution, and as an electron transporter, much lower electron injection barrier, slightly higher electron mobility and similar operational stability in the device, in comparison with those of Alq3.

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Improved field emission characteristics from yttrium oxide-coated single-walled carbon nanotubes

신민경, *이휘건

*한양대 자연과학대학 화학과 *한양대 화학과*

The field emission properties of yttrium oxide (Y_2O_3)-coated single-walled carbon nanotubes (SWNTs) were studied in a vacuum system. Yttrium oxide(Y_2O_3) fims have been deposited on SWNTs by magnetic sputtering. The SWNTs were dispersed in ethanol, dropped on a conductive Si wafer (100 miller index and 1–30Ωcm resistivity), and then dried. The experimental results show that the field emission current density increased and the turn-on field decreased more than pristine SWNTs. The maximum emission current density reached $1.19*10^{-4}$ A/cm^2, twelve times than that of pristine SWNTs $1.35*10^{-5}$ A/cm^2 at an electron field of 5.40 V/㎛. The turn-on field of pristine SWNTs decreased from 5.21 V/㎛ to 3.32 V/㎛ for yttrium oxide (Y_2O_3)-coated single-walled carbon nanotubes (SWNTs).

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Azido Gauche Effect on the Backbone Conformationof beta-Azidoalanine Peptides

오광임, 조민행

고려대 화학과

To study the azido gauche effect on the backbone conformation of beta-azidoalanine blocked dipeptide (AAD) and tripeptide (AAT), we used spectroscopic methods in combination of quantum chemistry calculations and molecular dynamics (MD) simulations. From the NMR studies, we found that AAD in water prefers the gauche− (g−) side-chain conformer and adopts either polyproline II (PPII) or C7 backbone conformation. From the amide I IR absorption and circular dichroism (CD) spectra, the backbone conformation of AAD in water is found to deviate from PPII, but rather close to C7. Likewise, 1H NMR data for temperature dependence and NOESY experiments bring the same information of conformations up. Thus, the backbone conformation of AAD differs from that of AD, which is mainly PPII in water. The underlying origin of the backbone conformational difference between AAD and AD in water was elucidated by using the quantum chemistry calculation results. From the electronic structure calculations with density functional theory (DFT), it was found that the C7/g− conformer is the lowest energy structure of an isolated AAD. Here, the beta-azido group forms intramolecular electrostatic interactions with two neighboring peptide bonds, which are facilitated by the azido gauche effect. Thus, the b-azido group appears to be responsible for directing peptide backbone conformation toward the C7 structure. The quantum mechanical/molecular mechanical (QM/MM) MD simulations show that AAD in water adopts neither PPII nor alpha-helix and prefers the g− conformer. Thus, the intramolecular electrostatic interactions between the beta-azido group and two nearby peptide bonds are also found even in the solution structure of AAD in water. Consequently, the beta-azido group appears to be an effective C7-conformation-directing element, which may also be useful for tuning the structures of other amino acids and polypeptides.

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Explicit solvent effect on the Tautomerizations of protonated 2-hydroxypyridine

Mohammad Harun, 최철호

경북대 화학과

The solvent water catalysis effects were studied on the tautomerization between protonated 2-hydroxypyridine (2HPH+) and protonated 2-pyridone (2PYH+). The protonation on nitrogen (2PYH+) yields much more stable isomer than on oxygen (2HPH+) by 40.2 kcal/mol. So it is clear that locally water autoinonized environment or acidic media strongly prefers 2PYH+ thermodynamically. The additional water significantly reduces tautomeric reaction barriers. Therefore, it is clear that in the dynamical solution media, even though the energetically less favorable 2HPH+ species can initially formed, it will soon be converted to the most stable 2PYH+, constituting thermodynamic controlled tautomerization of protonated species.

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Electric properties of TCNQ- and TTF- encapsulated single walled carbon nanotubes

박태희, 이휘건

한양대 화학과

Single-Walled Carbon nanotubes(SWNTs) have been found to be have a n-type transfer characteristics in vacuum. Reaction of single-salled carbon nanotubes (SWNTs) with molecules having large electron affinity and small ionization energy achieved p-type(TCNQ : Tetracyanoquinodimethane) and n-type(TTF : Tetrathiafulvalene) doping, respectively. Encapsulation of those molecules was carried out inside carbon nanotube under vacuum environment. The simplicity of the synthetic process offers a viable route for the large-scale production of SWNTs with controlled doping states, because of using mat-type SWNT. After encapsulation, TTF- and TCNQ-encapsulated SWNT deposited between electrodes of a bottom gate field effect transistor (FET) fabricated on Si-wafer substrate and investigate their electronic transport properties. FET character depends on changing gate voltages, Near IR and Raman were measured to elucidate charge transfer between those molecules and SWNTs.

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Field emission measurement of Carbon-nanotube peapods synthesized directly on Si substrates

이종택, 이휘건

한양대 화학과

Single-walled carbon nanotubes (SWNTs) encapsulating fullerenes, so-called "peapods," are attracting materials for electronics applications because of the interesting electronicproperty. To apply them to nano-electronics, it is important to develop a fabrication process. There are two methods in this process, synthesizing peapods directly on Si substrates and dropping peapods synthesized previously on substrates. To fabricate the devices, the former is more efficient than the latter. So we synthesize peapods directly on substrates. We use them in field emission, one of various application field. We study how much field emission of peapod directly on substrates enhances, and compare with results of dropping peapod and pristine SWNTs.

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Computational study on the enhancement of H_2 adsorption due to incorporation of Pd nanoparticles in NTB(4,4',4''-nitrilotrisbenzonate)

최성환, 정경준, 박지영, 이윤섭

KAIST 화학과

Spillover effect is one of the major ways to enhance hydrogen capacity. When hydrogen spillover occurs, hydrogen molecules dissociate and the atomic hydrogen migrate into metal organic framework. After the spillover, the binding type and the binding energy change compared to those before. Until now, there have been a limited number of studies on the hydrogen spillover phenomenon in ab initio approach. The hydrogen spillover is well known only in graphite, and not simulated in other substrates. Recently, the hydrogen spillover phenomenon was reported using the palladium nanoparticles in the porous material SNU-3, We try to understand the hydrogen spillover phenomenon in SNU-3 through quantum chemical calculations of the model system. We scan potential energy surface around the linker to locate the binding sites and energetics involved to demonstrate whether the spillover could be favored or not.

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Application of Isotope_Coded N-terminal Sulfonation to Study Ubiqitinated Peptides

장문석, 김인애, 이상원

고려대 화학과

Protein ubiquitination plays an important role in the degradation and other functional regulation of cellular proteins in organisms ranging from yeasts to mammals. Here we report the development of a novel strategy for searching ubiquitination site based on the N-terminal sulfonation. The sequence portion consists of an exclusive series of y-type ions and y' ions (differing by the loss of one glycine residue from the sulfonated Gly-Gly branch) that can directly reveal the amino acid sequence of the peptide and the precise location of the ubiquitination site. We present here a novel stable-isotope labeling method to simultaneously identify and quantify ubiquitin conjugated proteins produces Gly-Gly branched peptides by specifically derivatizing the N-terminus of proteins with 4-sulfophenyl isothiocyanate (SPITC). We describe the isotope coded N-terminal sulfonation (ICenS) of peptides; this procedure allows both de novo sequencing to be studied simultaneously. The experimental and ubiquitinated peptide mixture were derivatized independently using 13C-SPITC and 12C-SPITC and then combined to generate an isotopically labeled Gly-Gly branched peptides in which each isotopic pair differs in mass by 12Da. The 13C-labelled SPITC resulted inconvenient peptide pair spacing without isotopic overlap and hence facilitated relative quantification by LC-MS/MS. Our results show that the LC-MS/MS analysis of sulfonated peptides can provide a highly effective method for the determination of ubiquitination sites on protein targets, and modification sites on ubiquitins themselves.

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Selective Enrichment of Glycoproteins and Glycopeptides Using Boronic acid Functionalized Superparamagnetic Fe_3O_4@SiO_2 Nanoparticles

백승훈, 이상원

고려대 화학과

Glycosylation, a broad and biologically significant post-translational modification, is most commonly associated with secreted and membrane proteins. The discovery and identification of glycoproteomes, and the analysis of their glyco-structures are increasingly important in diagnosis and proteomics. Because of low abundance of glycopeptides, the enrichment step is needed for analysis of glycoproteomes. In this study, we focused on synthesis of 3-aminophenylboronic acid functionalized superparamagnetic nanoparticles and applying to selective separation of glycopeptides and glycoproteins. First, Fe_3O_4@SiO_2 nanoparticles (NPs) were coated 3-(Trihydroxysilyl)- propylmethylphosphonate (THPMP) and 3-aminopropyltriethoxysilane (APTS). Then, suberic acid bis(N-hydroxysuccinimide ester) is modified the surface of the Fe_3O_4@SiO_2 NPs coated with THPMP and APTS. Finally, 3-aminophenylboronic acid is modified the surface of the NPs. For the confirmation of the functionalized NPs, we experimented with SDS-PAGE using glycated BSA and glycated RNase and those proteins are successfully enriched by the NPs.

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Improved Performance and High Throughput in Proteomics Using Fast On-Line Enzyme Digestions and Targeted MS/MS with LTQ-FTICR

이정화, *Daniel López-Ferrer, 이상원

*고려대 화학과 *PNNL*

Protein digestion for bottom-up proteomics has traditionally been performed using a relatively lengthy incubation period (6-24 h). The proteomic digestion is one of the most time consuming steps in the analytical process and usually trypsin is the most widely used enzyme. However, it has an optimal activity at about pH 8 and below pH 7 the activity starts to drop off significantly. The performance of the pressurized systems, fast on-line digestion system (FOLDS), was demonstrated with pepsin for protein digestion in proteomics. Additionally, the use of targeted MS/MS method improved the quality of the data by at least in an order of magnitude. Therefore the coupling of FOLDS with a modified hybrid instrument improved the overall quality of the experiment in a reduced amount of time compared to standard protocols. Using this strategy we have been able to identify confidential peptides in a matter of minutes.

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Targeted Liquid Chromatography and Tandem Mass Spectrometry (LC-MS/MS) for High-throughput Proteomic Analysis based on integrated Post-Experiment Mass Filtering and Refinement (iPE-MMR)

박종문, 김호근, 형석원, 이정화, 이연화, *이후근, 이상원

*고려대 화학과 *가천의과학대 암당뇨연구원*

Despite of several efforts to obtain all MS/MS data of eluted species from liquid chromatography, this limitation still remains to overcome due to the high dynamic range of a given proteome sample. Targeted LC-MS/MS is a reasonable approach that allows selective identifications of peptides. Herein, we present targeted LC-MS/MS which is based on an intergrated Postexperiment Monoisotopic Mass Refinement (iPE-MMR) framework that contains a unique mass class (UMC) concept and monoisotopic mass filtering and refinement. The tryptic digests of 7 proteins were analyzed by fully automated ultra-high pressure liquid chromatography and fourier transformation ion cyclotron mass spectrometry (FT-ICR). The mass spectrometric data were treated by iPE-MMR method followed by sequest database search and then construction of peptide master map was conducted using those sequest results. The mass lists were constructed through the retention time and m/z of nonidentified unique mass classes (NonID UMCs) which are not matched with the peptide identifications in master map. As a result of this study, the number of collisional induced dissociation (CID) of ions in targeted mass lists was achieved up to 99% and totally 850 of peptides were identified.

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Investigation of Nucleosides-Copper complexes by electrospray ionization Mass Spectrometry

김미지, 정상미, 김호태

금오공과대 응용화학과

Z-DNA is a left-handed helix, with about 12 bp/turn, in contrast to the B-form right-handed helix characterized by 10.5 bp/helical turn. It is known that Copper(Ⅱ) ions play important roles to transform a general B-DNA to Z-DNA. However, several reports are not consistent with each other and that no clear agreement exists regarding the biological active structure of [Cu^{II}+base] complex during the biological process. In this study, we investigated the complex structures and binding sites of [Cu^{II}+CG] complex in gas phase by electrospray ionization mass spectrometry (ESI-MS) using 2'-Deoxycytidine (dC) and 2'-Deoxyguanosine (dG) for complex formation. MS/MS and MS/MS/MS fragmentation patterns of CG and [Cu^{II}+CG] complexes were analyzed by collision-induced dissociation (CID) method in an ion-trap LTQ mass spectrometer.

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Binding site analysis of Copper ion(Ⅱ)-Islet Amyloid Polypeptide(IAPP) complex by Electrospray Ionization Mass Spectrometry.

정상미, 임유진, 김호태

금오공과대 응용화학과

Amyloid deposits of IAPP in the pancreas are an important characteristic feature found in patients with Type-2 diabetes. It is generally accepted that the aggregated IAPP peptide is a cause for the loss of insulin-producing pancreatic β-cells in type 2 diabetic patients. Human IAPP is extremely amyloidogenic, while rat IAPP do not form amyloid in vitro or in vivo. It is known that a metal ion has an influence on aggregation of IAPP, and copper ion in particular inhibits the formation of IAPP amyloid. However, investigations regarding the $[Cu\text{Ⅱ}+IAPP]^{2+}$ complex have not been conducted systematically using MS. We present the result of the Ion-trap Electrospray Ionization(ESI) mass spectromerty(MS) study regarding the structure and formation process of copper ion-IAPP(human/rat) complex. The fragment patterns of $[Cu\text{Ⅱ}+IAPP]^{2+}$complex were analyzed by MS/MS and MS/MS/MS spectra in the gas-phase. As the results of MS/MS, MS/MS/MS is suggest to be binding site for the $[Cu\text{Ⅱ}+IAPP]^{2+}$ complex.

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Selective enrichment of phosphopeptides using superparamagnetic N-succinimidyl-3-(2-pyridyl dithiol)-propionate(SPDP) nano particles

정수라, 김가원, 백승훈, 김수진, 이광렬, 이상원

고려대 화학과

Phosphorylation is one of the post-translational modifications. Reversible phosphorylation plays an important role in regulating cellular processes. Because of the low abundance of phosphorylated peptides in protein and the negatively charged phosphate moiety, it is hard to analyze directly using mass spectrometry. So, the methods of modification and selective enrichment of phosphopeptides have been developed. The proton at α-carbon of phosphoserine was removed by β-elimination reaction with hydroxide, in which the phosphoserine was converted to dehydroalanine. Dehydroalanine was attacked by ethanedithiol(EDT) and became mercaptoethylcysteine. After modification, superparamagnetic 30 nm N-succinimidyl-3-(2-pyridyl dithiol)-propionate (SPDP) nanoparticles reacted with mercaptoethylcysteine to make a disulfide bond. With a magnet, peptides which had no site of phosphoserine were washed out and then the mercaptoethylcysteine peptides with nanoparticles were remained. The peptides with mercaptoethylcysteine were cleaved from nanoparticles by reduction and the thiol group on the mercaptoethylcysteine was protected by alkylation with iodoacetamide to prevent from disulfide bond between themselves. Through above methods, we successfully purified and enriched mono- and tetra-phosphopeptides.

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Breast Cancer Biomarker Discovery by Observing Phosphorylation Site Change Accompanied by TGF-β Treatment and Mutation Gradient

마경진, *이후근, 이상원

*고려대 화학과 *가천의과학대 암당뇨연구원*

Since breast cancer is relatively easy to be removed than cancer on other organs, early diagnosis of breast cancer can prevent metastasis and save plenty of patients. Phosphorylation known as a regulator of cellular processes causes or prevents the mechanisms of diseases such as cancer and diabetes. In other words, phosphorylation can be the key for finding biomarkers for early diagnosis of breast cancer. The TGF- β affects complicatedly in carcinogenesis since it plays as either a tumor suppressor or a pro-oncogenic pathway. For the purpose of understanding how TGF- β (Transforming Growth Factor-beta) affects to phosphorylation site on breast cancer cell line, MCF10A, we treated TGF-β during cell culture. To analyze phosphopeptide with mass spectrometer, enrichment step is necessary in complex sample. We applied IMAC and TiO2 to same sample as enrichment methods complementally. By the treatment time difference, mutation gradient and difference of enrichment methods, we got 24 samples. Search process was delivered by two search engine, SEQUEST and X!tandem in terms of complemental ways after LC/MS/MS experiments. 1000 nr peptides and 350 phosphopeptides were detected in 24 samples on the average. We used postexperiment monoisotopic mass filtering and refinement (PE-MMR) method developed for label free quantification. Mass calibration and retention time normalization was conducted for it. Retention time normalization process was performed by the method from PNNL. TGF-b signaling pathway is visualized with Cytoscape.

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Experimental and Theoretical Investigations of the photodissociation dynamics of Substituted Thioanisoles

윤준호, *김상규

*KAIST 화학 *KAIST 화학과*

We compare recoil energy distributions and anisotropy parameters(β) of thioanisole(TA) and substituted analogs[4-XTA, X=F (1) and CH3 (2)] at the para position using velocity mapped ion imaging. The X/A branching ratio is estimated from the total translational energy distribution to find the energetic location of the S1/S2 conical intersection (CI). It shows chemical substitution at the para position of TA significantly changes the dynamics in the vicinity of the CI. We observed a remarkable fano resonance at the CI only for the TA. For other molecules, it is hard to reach the CI energetically in the Franck-Condon region due to the significant change of dynamics. Energy gap between the A and X state of XC6H4S radical which is essential for so-called intramolecular orbital alignment is calculated using the complete active space second-order perturbation theory (CASPT2). It shows the substituted analogs have increased energy gap and the substituent effect is explained using a simple molecular orbital theory. We plan the adaptation of the multistate second-order perturbation theory at the optimized CI geometries to explain the photodissociation dynamics of substituted thioanisoles.

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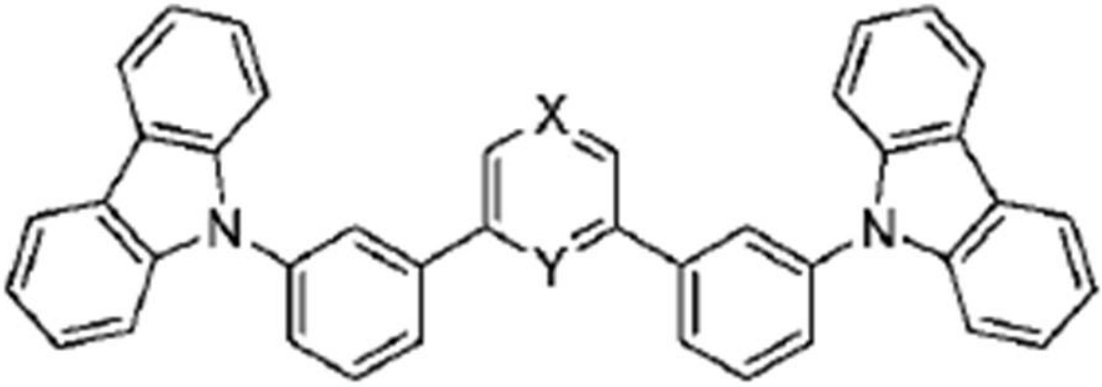
Theoretical investigation of pyridine-containing carbazole derivatives as ambipolar host materials for blue electrophosphorescence

김동욱

경기대 화학과

Recently, blue organic light-emitting diodes of the highest efficiency (higher than 20% and 34lm/W) has been developed by employing as hosts pyridine-containing carbazole compounds, 2,6-bis(3-(carbazol-9-yl)phenyl)pyridine (26DCzPPy) and 3,5-bis(3-(carbazol-9-yl)phenyl)pyridine (35DCzPPy).1 These compounds were designed to be ambipolar host materials by integrating pyridine unit for efficient electron injection/transfer with carbazole units for facile hole injection/transfer and high triplet energy. However, a theoretical study uncovers that the lowest triplet energies of these compounds are governed by the phenyl-pyridine bridge rather than carbazole unit. Furthermore, experiments also indicated that exciton formation may not be important such that the exciton formation of the light emitting guest may more likely be achieved by charge transfer from the host rather than direct energy transfer from the host to the guest. This aspect will also be addressed on the basis of calculational results.Reference1. Su, S.-J.; Sasabe, H.; Takeda, T.; Kido, J. Chem. Mater. 2008. 20. 1691



26DCzPPy X=CH, Y=N
35DCzPPy X=N, Y=CH

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Study on hybrid plasma-polymer thin films of different ratio between toluene and TEOS for low dielectrics

조상진, 부진효

성균관대 화학과

Organic-inorganic hybrid co-polymer thin films were deposited on silicon(100) substrates under the several ratio of TEOS (tetraethoxysilane) against toluene by plasma enhanced chemical vapour deposition (PECVD) method. Toluene and TEOS were utilized as organic and inorganic precursors each, and hydrogen and argon were also used as a bubbler and carrier gases, respectively. In order to compare the difference of the electrical and the mechanical properties of the plasma polymerized thin films, we grew the hybrid co-polymer thin films under the conditions of various ratio between toluene and TEOS with fixed RF (radio frequency using 13.56 MHz) powers at 30 W. The as-grown polymerized thin films were in first analyzed by FT-IR and XPS. The result of FT-IR showed that the co-polymer thin films were polymerized with fragmented each precursor. Also, XPS results showed the chemical speciesand binding energies of each species. Si 2p core-level spectra from the hybrid polymer thin film showed the status of Si oxidation number. Impedance analyzer was utilized for the measurements of I-V curves and capacitance values. Also, the thin films were analyzed for hardness and Young's modulus by nano-indenter.

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Hydrophilicity of TiO_2 thin films obtained by thermal chemical vapor deposition

최진우, 부진효

성균관대 화학과

We have deposited nano-crystalline hydrophilic TiO_2 films on slide glasses using titanium tetraisopropoxide (TTIP) as a precursor by metal-organic chemical vapor deposition (MOCVD). The temperature of substrate was 400 °C and the temperatures of precursor were kept at 75 °C (sample A) and 60 °C (sample B) during the TiO_2 film growth. The deposited TiO_2 films were characterized by contact angle measurement and uv/vis spectroscopy. The results show that sample B has very low contact angle of almost zero due to superhydrophilic TiO_2 surface and transmittance is 76.85 ± 1.47 % at the range of 400 – 700 nm. So, this condition is very optimal for hydrophilic TiO_2 film deposition. However, when the temperature of precursor is lower than 50 °C or higher than 75 °C, TiO_2 could not be deposited on the substrate and cloudy TiO_2 film was formed due to low precursor temperature and the increase of surface roughness, respectively.

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Uniaxial Tip Pressurizing Can Modulate Charge Transfer : The Role of Interconnection Between Metal Surface and Molecule Probed via Surface-Enhanced Raman Scattering (SERS)

박원화, 김지환

고려대 화학과

Utilizing local "tip-pressure" as an experimental variable onto the individual metal nanoparticle-4-aminobenzenethiol (ABT)-metal plane junctions enables us to explore the charge transfer (CT) in the SERS of non-resonant molecules. First of all, we observe overall SERS intensity decline upon uniaxial tip pressurizing onto the isolated Ag nanoparticle-ABT-Au plane junctions, which may be interpreted as *plasmonic quantum mechanical tunneling* with sligh molecular lateral diffusion within local eletromagnetic(EM) field region. In particular, the observed *"mode-specific"* SERS intensity decrease of ABT allows us to claim that the intentional dissociation of ionic bond between metal surface and amine group by employing uniaxial tip pressure may play a role in modulating CT-activity. Detailed and more quantitative comparison of SERS intensity between 4-aminobenzenethiol and 4-methyl benzenethiol with same metal (Au,Ag) nanoparticle-plane hot spot system strongly substantiates the importance of chemical (electronic) interaction between metal surface and molecules by *through bond-CT* mechanism in terms of yielding mode-selective SERS enhancement.

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Enantioseparation on cellulose tris(3,5-dimethylphenylcarbamate)-coated zirconia monolithic columns by capillary electrochromatography

박정학, **AVVARU PRAVEEN KUMAR**, 김은주, 김민지, 홍종성

영남대 화학과

This work reports the preparation of monolithic zirconia chiral columns for separation of enantiomeric compounds by capillary electrochromatography (CEC). Using sol-gel technology a porous zirconia monolith of interconnected skeleton structure with through pores was synthesized in the capillary column, and then the surface of the monolith was coated with cellulose tris(3,5-dimethylphenylcarbamate) (CDMPC) to obtain a monolithic chiral column (CDMPCZM). The process of the preparation of the zirconia monolithic column was investigated by examining the effects of concentration of the components of the sol solution composed of zirconium n-butoxide, polyethylene glycol, water and acetic acid on the formation of porous zirconia monolithic structure. The EOF and enantioseparation behavior of a set of racemic analytes on CDMPCZM were investigated in RP mobile phases of varying pH, organic composition and applied voltage.

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Structural identification of heavy components of crude oil by ion mobility mass spectrometry

조윤주, 김성환

경북대 화학과

Next stage of petroleomic research needed to move forward is structural elucidation of the identified compounds. With recent advance of thchnology, ion mobility separation with higher resolution can be achieved to separate and identify ions based on their collisional cross section or structures. However, it is not trivial to separate and study individual ions because of petroleum's complexity. Therefore, ion mobility mass spectrometry coupled with ASAP ionization source was used to study petroleum samples. Two oil samples and their toluene and heptanes soluble fractions were analyzed by SYNAPT G2 mass spectrometer coupled to atmospheric solids analysis probe(ASAP) source. Here, oil samples were provided by SK Energy Corporation and SYNAPT G2 mass spectrometer(Manchester, England) was used for data acquisition. MassLynx with driftscope 2.0 software was used for the data analysis. The spectra were obtained with the probe temperature set at three temperatures,200,400,and 650 ℃. The mass spectrometer was operated with V mode to achieve better mass accuracy and resolution. As a result, the thousands of peaks separated by drift time and m/z were obtained. The obtained peaks were divided into even and odd ions to reduce the complexity. Subsequent data analysis showed that the peaks differing either by H_2 and CH_2 had their own specific slopes in the drift time vs m/z plot.

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Linker effect on the electronic structure & catalytic activity in metal-CNT nanocomposites.

김자영, 최현철

전남대 화학과

Carbon nanotubes (CNTs) have drawn particular attention on account of both their scientific interest and their potential for technological applications. Recently, CNTs are receiving considerable attention as catalyst supports due to their high mechanical strength, large surface area, good electrical conductivity, and durability under harsh conditions. Some researchers have reported that CNT supported catalysts (e.g., Pt, Pd, Au, Ru and RuO2) exhibited good catalytic behaviors in various chemical reactions, involving methanol electro-oxidation, selective hydrogenation, alcohol oxidation, Suzuki coupling, CO oxidation, and hydrodehalogenation. A simple method of depositing Pd nanoparticles onto CNTs as catalyst supports is devised for C-C bond forming reactions. Thiol groups were utilized as linkers to secure the Pd nanoparticles without agglomeration. In the present study, we investigated linker effect on the catalytic activities using the different thiol compounds. This result indicates that surface thiolation is an effective way to obtain highly dispersed metal nanoparticles on the surface of CNTs and markedly improves their catalytic activity.

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Synthesis of carbon nanotube supported Pd catalysts and evaluation of their catalytic behavior for C-C bond forming reactions.

김자영, 최현철

전남대 화학과

Carbon nanotubes (CNTs) are receiving considerable attention as catalyst supports in both heterogeneous catalysis and electrocatalysis due to their high mechanical strength, large surface area, good electrical conductivity, and durability under harsh conditions. Some researchers have reported that CNT supported catalysts (e.g., Pt, Pd, Au, Ru and RuO2) exhibited good catalytic behaviors in various chemical reactions, involving methanol electro-oxidation, selective hydrogenation, alcohol oxidation, Suzuki coupling, CO oxidation, and hydrodehalogenation. One of the most important issues in current organic synthesis is the development of new efficient carbon-carbon and carbon-heteroatom bond forming reactions. In this work, we report a simple and effective process to prepare CNT-Pd nanocomposites by depositing Pd(dba)2 on thiolated multiwall carbon nanotube (MWNT) surfaces. A high-yield C-C bond forming reaction accomplished at a low Pd content (~ 2.0%) and in the absence of any ligand is observed. This synthetic approach should be broadly applicable for preparing CNT-supported metal catalysts and markedly improves the catalytic activity.

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Reactive gas effect on detection of explosives by ion mobility spectrometry with corona discharge ionization source

김윤기, 최성신, *신명원, *최규섭, *맹석진, *안승건

*세종대 화학과 *(주)우주씨앤티 기술연구소*

The increasing worldwide terrorist threats nowadays have made it crucial to detect all kinds of explosives in order to provide a secure protection for important places such as air ports, embassies, governmental buildings, public and holy places, power stations, dams, etc. Many methods have been reported for the detection of explosives and various techniques have been comprehensively reviewed in the literature. X-ray screening, fluorescence quenching, neutron and gamma-ray spectroscopy, LC–MS, UV gated Raman spectroscopy, laser induced breakdown spectroscopy (LIBS), electrochemical and immunosensors, chemiluminescence, SPME-HPLC, and GC-ECD are new methods proposed for explosive detection. Ion mobility spectrometry (IMS) has proved to be one of the best methods for the detection of trace level of explosives due to its low detection limit, fast response, simplicity, and portability. IMS-based instruments are now vastly used in vulnerable places such as airports for screening of both people and carry-on luggage. In this study, IMS equipped with corona discharge ionization source was constructed and its performance was tested with various explosives. Furthermore, we studied reactive gas effect for various explosives.

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Analysis of residual monomers in ABS using gas chromatography

김윤기, 최성신

세종대 화학과

Poly(acrylonitrile-co-butadiene-co-styrene) (ABS) is a common thermoplastic used to make light, rigid, and molded products such as piping, automotive body parts, protective headgear, toys, and food containers. The nitrile groups of ABS attract each other and bind the chains together, making ABS stronger than pure polystyrene. The styrene gives shiny and impervious surface. The butadiene, a rubbery substance, provides resilience even at low temperatures. During the production of ABS, a small fraction of unreacted monomers such as acrylonitrile, styrene, and 1,3-butadiene can be physically entrapped in the polymer. As regards toxicity, the residual monomers are classified as a carcinogen or a mutagen. In this work, the level of residual monomers in ABS are determined by gas chromatography (GC) with flame ionization detection(FID). Headspace and liquid samplings were employed as a sample injection method and the results were compared.

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Analysis of alkylphenolic resole resin by MALDI-TOFMS

정혜승, 최성신

세종대 화학과

Alkylphenolic resins are divided into resole resin and novolack resin according to the reaction conditions. Alkylphenolic novolack resin is made by reaction of excess alkylphenol with formaldehyde in acidic condition and mainly used as adhesives. On the other hand, alkylphenolic resole resin is made in basic condition and used as crosslinking agents. The linkages between the alkylphenols are dimethylene ether (-CH2OCH2-) and the methylene (-CH2-). Since the alkylphenolic resoles are used in crosslinking agents, their molecular weight distribution and presence of functional groups are very important. Until now alkylphenolic resole resins have been analyzed by FTIR, HPLC, GPC, pyrolysis, and TGA. The matrix-assisted laser desorption/ionization–time of flight mass spectrometry (MALDI-TOFMS) method can be successfully applied the measurement of exact molecular weight. In this study, we examined microstructures of alkylphenolic resole resin by MALDI–TOFMS.

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Analysis of alkylphenol-formaldehyde resole resin by APCI-MS

김옥배, *최성신

*세종대 응용화학과 *세종대 화학과*

Alkylphenol-formaldehyde resole resin is made by reaction of alkylphenol with excess formaldehyde in basic condition. Resol resin is generally used as crosslinking agents of rubber and its property is determined by the kinds of linkages (methylene or dimethylene ether) and end groups (hydrogen or methylol). HPLC, GPC, IR, NMR, and MALDI-MS have been employed to analyze phenolic resins. HPLC and GPC do not give structural information of an analyte, while IR and NMR are good analytical methods but the molecular weight distributions cannot be determined using them. Atmospheric pressure chemical ionization-mass spectrometry (APCI-MS) is a suitable analytical method to determine both molecular weight and functional group of resol resin. In this study, we examined microstructures of alkylphenol-formaldehyde resol resin by APCI-MS.

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Amperometric Proton Selective Sensors based on Facilitated Ion Transfer Reactions at Liquid/Liquid Interfaces

Shaikh Nayeem Faisal, 권민정, 이혜진

경북대 화학과

In this poster, we demonstrate a cost-effective amperometric proton selective sensor based on facilitated proton transfer reactions by proton selective ionophores across a polarized micro-interface between the aqueous phase and the polyvinyl chloride-2-nitrophenyloctylether (PVC-NPOE) gel phase. A single micro-hole interface was fabricated by simple mechanical punching with sharp needles on a thin PVC film (12 μm thick) commercially available as a food wrapping material. In order to enhance the selectivity of proton sensing, two different proton selective ionophores (i.e. dibenzo-18-crown-6 and octadecyl isonicotinate) were introduced into the organic gel layer and their electrochemical sensing characteristics were studied using cyclic voltammetry and differential pulse stripping voltammetry. The resulting amperometric sensors show good sensitivity towards different concentrations of hydrogen ions.

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Attomolar Detection of Proteins using Gold Nanorod-enhaced Surface Plasmon Resonance

심혜림, 남은지, 이혜진

경북대 화학과

In this poster, we present an ultrasensitive detection method for protein biomarkers using biofunctionalized gold nanorods in conjunction with surface plasmon resonance (SPR). As a model protein marker, immunoglobulin E was selected because the protein has two different binding sites, anti-IgE and IgE specific aptamer, which can provide a direct sandwich detection platform without labeling target proteins with amplification tagging molecules. The surface sandwich complex was created by the adsorption of IgE onto the surface immobilized IgE-aptamer followed by the adsorption of anti-IgE coated gold nanorods. Attomolar concentrations of IgE could be directly detected, which is an extraordinary 1,000,000 improvement compared to that of using a conventional SPR detection based on the direct measurement of IgE protein binding onto the surface bound IgE-aptamer.

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Application of Solid-State Carbon-13 NMR Spectroscopy to Study SOM Processes

오세웅, *H. A. Enloe, **S. A. Quideau, **R. E. Wasylishen

*목포대 화학과 *University of California, U.S.A. **University of Alberta, Canada*

Solid-state Carbon-13 NMR spectroscopy was used to gain insight into soil organic matter accumulation and decay processes within two arboreal soils. Arboreal soil, redwood and fern litter as well as epiphyte roots were analyzed. Carbon-13 NMR spectroscopy analyses resulted in a preferential decomposition of carbohydrates and an accumulation of alkyl structures from the redwood and fern litter to the

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Sample cleanup and preconcentration for capillary electrophoresis-mass spectrometry using single drop microextraction and large volume sample stacking

김지혜, 최기환, 정두수

서울대 화학부

Single drop microextraction (SDME) and large volume stacking using an electroosmotic flow pump (LVSEP) were coupled to capillary electrophoresis-electrospray ionization-mass spectrometry (CE-ESI-MS) for sample cleanup and preconcentration before and after sample injection. SDME was performed with a pentanol drop (as an organic solvent) at the tip of a fused silica capillary, which was immersed in the aqueous donor phase. A Teflon tubing sleeve was placed around the inlet capillary as a hydrophobic support. After SDME, the capillary was filled with the enriched pentanol extract and then further concentrated by LVSEP. In LVSEP, the adverse effects of a long sample matrix plug were overcome by pumping the plug out of the separation capillary to the inlet vial using the electroosmotic flow under a potential of reverse polarity. Therefore, for the drop formation and the sample matrix removal, it was necessary to supply a backup run buffer from the outlet and of the capillary, which was not trivial in most CE-MS system. We solved this difficulty simply by placing a vial supplying a backup run buffer during the drop formation and matrix removal processes without any physical modification of a conventional sheath liquid CE-ESI-MS interface. After the double sample preconcentration by SDME and LVSEP, several hundred-fold enrichments were achieved for anionic analytes including chlorophenols.

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Determination of Concanavalin A Based on Catalyzed Luminol Reaction

권진주, 이원용

연세대 화학과

Specific binding of carbohydrate and lectin on the cell membrane is important in cell recognition and cell signaling pathway. Thus, study on the interaction between carbohydrate and lectin makes one find out the mechanism of the reaction on the cell surface. Method of lectin determination is expected to be an useful tool for the study. This research suggests a luminol electrochemiluminescence (ECL) method to determine concentration of concanavalin A. Concanavalin A is lectin specifically bound to mannose. The thiol-derivatized mannose is self-assembled on the gold electrode and then, combines with the Con A of sample solution. The colloidal gold-labeled mannose combines with the Con A fixed on the gold electrode. Through this process, signaling molecule is also fixed on the gold electrode. The signaling molecules catalyze luminol ECL. By measuring the luminol ECL intensity, concanavalin A concentration can be determined.

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Lipid Profiling in Lipoproteins from Controls and Patients with Coronary Artery Disease by Flow Field-Flow Fractionation and NanoflowLC-ESI-MS-MS

이주용, 문명희

연세대 화학과

Principal function of Lipoprotein is to transport lipids through vascular and extra vascular body fluids. Lipoproteins are macromolecular assemblies of lipids and proteins and they are classified according to their densities into three different categories : high-density lipoprotein (HDL), low-density lipoproteins (LDL), very-low-density lipoproteins (VLDL). Among them, variations of size, density and composition of LDL are deeply related to Coronary Artery Disease (CAD). Flow field-flow fractionation (FlFFF), a separation technique for nanosized materials, was utilized for selective detection and separating lipoprotein particles stained by using Sudan Black B and NBD ceramide. In FlFFF channel, separation of particles or macromolecules is carried out bv the difference in diffusion coefficients of particles. With FlFFF, comparison of size distribution between controls and CAD patient samples was studied by asymmetrical FlFFF (AFlFFF), and their lipoprotein particles from the blood plasma were fractionated by multiplexed hollow fiber FlFFF (MxHF5).Phospholipids of fractionated lipoproteins were analyzed by nLC-ESI-MS-MS. In this study, five classes of phospholipids (phosphatidyl choline, phosphatidyl ethanolamine, phosphatidyl glycerol, phosphatidyl inositol, phosphatidic acid) were analyzed.

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Quantitative Analysis of Human Urinary Phospholipids from patients with prostate cancer using nano-flow LC-ESI-MS-MS

민혜경, 문명희

연세대 화학과

Phospholipids are the main constituents of biological membranes and have important structural and functional properties. Based on differences in their polar head groups, the phospholipids are divided into several classes. Phospholipids also play a main role in signal processing and as precursors for many other biologically vital molecules. Traditionally, phospholipids extracted from biological samples have been separated by thin-layer chromatography(TLC), gas chromatography(GC), however this method was relatively complicated and time consuming. Alternatively phospholipids could be analyzed by HPLC with UV absorbance or evaporative light scattering detection. But this method has a poor selectivity, therefore identification of the various molecular species must be realized by the comparison of their retention behavior with that of known standards. Recently analysis of phospholipids derived from biological sources has been achieved through exploiting the high-efficiency volatilization of phospholipids by electrospray ionization mass spectrometry. The main phospholipids extracted from human urine were analyzed by reverse-phase nano-flow liquid chromatography coupled with electrospray ionization (ESI) ion-trap mass spectrometry (MS). By using a C18 column and gradient of water/acetonitrile/isopropanol as mobile phase containing formic acid(using positive ion mode)/ammonium hydroxide(using negative ion mode) as modifiers. Phosphatidyl choline(PC), phosphatidyl ethanolamine(PE) were detected at positive ion mode, phosphatidyl serine(PS), phosphatidyl inositol(PI), phosphatidyl glycerol(PG), phosphatidic acid(PA) were detected at negative ion mode. Quantitative analysis of phospholipids is performed using internal standards (16:0/16:0 PE 0.5pmol) for compensation of ionization efficiency of MS detector. In this study, human urinary PLs of prostate cancer are characterized quantitatively.

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Separation of phospholipids by Monolithic Open-Tubular Capillary Electrochromatography with Electrospray Ionization Mass Spectrometey(OT CEC-ESI/MS)

장린, *정원조, 문명희

*연세대 화학과 *인하대 화학과*

Phospholipids(PLs) are major component of cellular membrane as they form double layer structure of membrane and play important roles in signal transduction. While thin layer chromatography and HPLC are currently utilized for the analysis of PLs, there is always a need to develop a new method with high speed separation as well as the minimized usage of organic solvents. In this study, capillary electrochromatography(CEC) has been tested as an alternative method for the separation of phospholipids in combination with on-line ESI-MS-MS. Implementation of OT(Open tubular) column with the help of electroosmotic flow can be an alternative to improve LC separation in monolithic open tubular capillary electrochromatography(OT-CEC). Currently, separation of phospholipids with capillary zone electrophoresis can not be obtained by the differences in the length and unsaturation degree of acyl chain of PLs, but only by the differences of head groups. When used with open-tubular column in this study, we have demonstrated that PLs can be separated not only by head groups, but by the variation in acyl chain. In addition, we developed a simple inexpensive CEC-ESI-MS interface using a coaxial sheath flow in the laboratory incorporated with a simple Tefzel cross. For the performance test of the interface, several peptides were separated and detected by the on-line connection with ESI-MS.

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Recovery Enhancement of Proteome Separation in Hollow Fiber Flow Field-Flow Fractionation by Using Surfactant

김기훈, 문명희

연세대 화학과

Human serum is complex fluid from body that contains various proteome involved in many diseases. However some major proteins like human serum albumin cause an interference of analysis by mass spectrometry, so proper separation technique is required previously. Hollow fiber flow field-flow fractionation (HF5) has been demonstrated as a tool for pre-fractionating proteomes by differences in hydrodynamic diameter (ds), where the resulting protein fractions can be analyzed after digestion by shotgun proteomic method using nanoflow chromatography-electrospray ionization-tandem mass spectrometry (nano LC-ESI-MS/MS). In this study, SDS solution was utilized to increase recovery of proteome smaller than pore size of Hollow Fiber membrane (< 30 kDa) by inducing SDS-protein complexes. Since molecular size of induced complexes are enlarged, their elution can be increased in HF5 separation. Additionally, subunits of some proteins were also fractionated. We observed the change of retention time and peak area of some standard proteins and applied this method to human serum proteome.

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Profiling of Phospholipids from Prostate Cancer Cell lines treated with Allose Using Nano-flow LC-ESI-MS/MS

정래웅, 문명희

연세대 화학과

Lipidomics research involves the profiling and quantification of the thousands of cellular lipid molecular species and their interactions with other lipids, proteins, and other metabolites. Among the complicated lipid molecules, phospholipids (PLs) have a majority of lipids, about 70%, that constitute cell membranes. In this study, nanoflow liquid chromatography coupled with electrospray ionization tandem mass spectrometer (LC-ESI-MS/MS) was employed for the analysis of phospholipids mixture in prostate cancer cell line (PrEC, DU145, LNCaP) that were treated with allose. Allose is an aldohexose sugar and antineoplastic material that is under investigation of its effect on cancer development. Separation of phospholipids are carried out using a home made reversed phase capillary column with a pulled tip and the MS experiment of eluted phospholipids is performed at the precursor scan first and followed by data dependent MS/MS scan. Qualitative analysis of phosphatidylcholines and phosphatidylethanolamines for the cancer cell lines with or without treatment of allose is carried out and the differences of the distribution of the identified PLs are compared in this study.

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Effect of Asymmetrical Flow Field-Flow Fractionation Channel Geometry on Separation Efficiency

안지연, 이주용, 문명희

연세대 화학과

Flow Field-Flow Fractionation (FlFFF) is the most versatile method among the various FFF techniques. FlFFF using asymmetrical channel, called Asymmetrical FFF (AFlFFF), has an inlet flow, which serves as a source for both the migration flow along the channel length and cross-flow through the permeable wall. Molecules are separated by these two flows, but there is an axial velocity gradient that affects the separation capability in asymmetrical channel design. By calculating this gradient, it is already known that a trapezoidal channel has smaller gradient than a rectangular channel. However, the minimized gradient of trapezoidal channel is not sufficient to provide a constant velocity. That is, it additionally requires nonlinear decrease of the breadth. An exponential channel can help us to get the constant mean channel velocity. We designed a series of channels suggested by an earlier theoretical development in literature. We tested the exponential channel with polystyrene(PS) latex particles from 20nm to 135nm, by only changing the channel geometry. The rectangular channel results in a serious band broadening due to decreasing mean flow velocity along the channel continuously. The trapezoidal channel performs as a reliable tool in reducing the serious band broadening. However the exponential channel performs better in reducing band broadening and in terms of operating at different flow rate conditions too.

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Validated resolution of thyroxine enantiomers in plasma using a crown ether derived chiral stationary phase by HPLC

이원재, 황호, 전소희

조선대 약학대학

It was demonstrated that the simultaneous determination of D-thyroxine (T4) and L-T4 on a chiral crown ether derived column in human plasma with base-line separation. This new analytical method for the determination of D-T4 and L-T4 using internal standard has been developed and validated. Validation experiments have shown that this method has good precision and accuracy as well as high linearity of 0.9987 and 0.9996 for D-T4 and L-T4 over the concentration ranges of 1-100μg/mL, respectively. This new analytical results using the chiral HPLC column may be used to investigate not only the simultaneous determination of D-T4 and L-T4 for biological samples but also the degree of conversion of each T4 enantiomer in vivo.

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Preparation of Pd decorated carbon nanotubes and evolution of their electrochemical properties

정유나

전남대 자연과학대학 화학과

Carbon nanotubes (CNTs) are considered as a novel nano-sized material playing a vital role in the field of nanotechnology. One of the main promising properties of CNTs is that it can enhance the electron transfer between the electroactive species and the electrodes. With the subtle electronic properties, the CNTs as an electrode material have been studied in detail and can be used in electrochemical sensing. In this study, Pd nanoparticle decorated CNTs were prepared using thiolated CNT by conventional reducing method. The prepared Pd-CNT nanocomposites are characterized using various analytical techniques like SEM, TEM and FT-IR spectroscopy. The presence of Pd nanoparticles is confirmed by XPS analysis. The prepared Pd-CNT electrode is utilized for investigating the electrooxidation of formic acid and formaldehyde. Electrochemical behaviors were also compared with the reference systems.

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New type stationary phase prepared by polymerization of styrene on initiator-attached monolith particles.

이승미, 정원조

인하대 화학과

In this work, initiator bonded monolith particles have been prepared and used to make a new stationary phase by radical polymerization. First, silica monolith particles were obtained from the polymerization product prepared by heating the reaction mixture of tetramethylorthosilicate (TMOS), polyethylene glycol(PEG), and acetic acid. The monolith silica particles were reacted with (3-choloropropyl) trimethoxysilane followed by sodium diethyldithiocarbarmate to make initiator attached silica monolith particles. The dried initiator monolith particles were then allowed to undergo radical polymerization with styrene to give a new stationary phase. The new stationary phase was packed in a microcolumn to examine its separation performance. The results were satisfactory. We were able to attain the numbers of theoretical plates up to 30.000.

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Direct Visual Detection of DNA Based on the Light Scattering of Silica Nanoparticles on a Human Papillomavirus DNA chip

piao jing yu, 정두수

서울대 화학부

A detection system for a human papillomavirus (HPV) DNA chip based on the light scattering of aggregated silica nanoparticle probes is presented. In the assay, a target HPV DNA is sandwiched between the capture DNA immobilized on the chip and the probe DNA immobilized on the plain silica nanoparticle. The spot where the sandwich reaction occurs appears bright white and is readily distinguishable to the naked eye. Scanning electron microscopy images clearly show the aggregation of the silica nanoparticle probes. When three different sized (55 nm, 137 nm, 286 nm) plain silica nanoparticles were compared, probes of the larger silica nanoparticles showed a higher scattering intensity. Using 286-nm silica nanoparticles, the spots obtained with 200 pM of Target DNA were visually detectable. The demonstrated capability to detect a disease related target DNA with direct visualization without using a complex detection instrument provides the prerequisite for the development of portable testing kits for genotyping.

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The Analysis of streptomycin residues in Surface water and drinking water by Liquid chromatography-tandem mass spectrometry

이종혁, 명승운

경기대 화학과

Streptomycin(STR) is an aminoglycoside antibiotic which in used in medical and animal origin, like meat, milk and honey widely. The method for the determination of streptomycin in surface water and drinking water by LC/ESI-MS/MS was developed. After ion pairing reagent was added, aqueous samples were extracted and concentrated through a Hydrophilic-Lipophilic Balance (HLB). In reverse phase liquid chromatographic (RPLC) system, chromatographic separation was achieved on a Eclipse Plus C18 column (2.1x100 ㎜, 5 ㎛), using gradient elution with 20mM HFBA in water and acetonitrile. After HPLC separation, quantification and qualification were performed by electrospray ionization(ESI) and tandem mass spectrometry. As a result, calibration curve showed good linearity (above r2=0.99) in the concentration range of 0.05~2.0 ㎍/L. From the spiked surface water, the limit of detection (LOD) and the limit of quantitation (LOQ) were 0.07 ㎍/L and 0.23 ㎍/L, respectively and recovery was the range of 48.7～76%. And from the spiked drinking water, the limit of detection and the limit of quantitation were 0.01 ㎍/L and 0.05 ㎍/L, respectively and recovery was the range of 58.1～105.5%. The established method can be used to determine ㎍/L levels of streptomycin from the environmental aqueous sample.

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Simultaneous analysis of six pharmaceuticals in soil and sediment by LC/ESI-MS/MS

김병주, 조현우, 명승운

경기대 화학과

The occurrence of pharmaceuticals in the environment is a growing concern. Pharmaceutical ingredients, including their metabolites and conjugates, are mainly excreted in urine or feces. Therefore, it required rapid and certain analytical method for pharmaceuticals which are existed in environment. In this study, sample preparation and analytical method for a monitoring of pharmaceuticals from soil and sediment were investigated. The extraction and clean-up of pharmaceuticals from soil were performed by HLB(Hydrophilic-Lipophilic Balanced) cartridge and solvent. The method provides for the simultaneous determination of six pharmaceuticals (iopromide, cefadroxil, cephardine, penicillin G, vancomycin and fenbendazole) by HPLC/ESI(+)-MS/MS. Recoveries of the pharmaceuticals were between 62.3 to 90.5% (except fenbendazole) and the overall variability of the method was below RSD 14.5%. The calibration curves showed good linearities (above r2=0.99) in the concentration range of 0.08~5.0 μg/kg. The limit of quantification (LOQ) were between 0.22 and 2.57 μg/kg. This analytical method are useful for the analysis of the pharmaceutical in soil and sediment.

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Development of optical and electrochemical sensors by a sol-gel derived glass matrix

김동완, 황재영, 최명룡, 김재상

경상대 화학과

To obtain selective glass membrane electrodes for anions and cations, pH electrode glass membranes were modified by a sol-gel method using a alkoxysilyl quaternary ammonium salts and salophen/salophen-metal complexes. Self-assembled monolayers (SAMs) modified sensors exhibit unique behavior that can greatly benefit optical and electrochemical sensing. This paper reported the different optical and electrochemical systems of sol-gel derived glass matrix for detecting inorganic and organic species.

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Fluorescent Sensor for Dicarboxylate Based on Organo-palladium Complexes in a Polymeric Film

김동완, 황재영, 김정환, 김재상

경상대 화학과

A new optode membrane for the sensitive and selective determination of dicarboxylate ion(maleate, fumarate, phthalate, telephthalate, etc) based on a change in the absorption spectrum of a polymer film, is proposed. A membrane composed of plasticized poly vinyl chloride (PVC), an dichloro-palladium complexes with terthiophene oligomer as a chromoionophore and a additive(TDMAC) was prepared. The influence of different plasticizers was studied concerning the sensitivity, linear range and selectivity of the membrane film. Satisfactory analytical sensing characteristics for determining dicarboxylate ion were obtained in terms of the selectivity, reversibility and reproducibility with a good detecting range.

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The Simultaneous Analysis of Macrolides in treated drinking water by LC/ESI-MS/MS

박미선, 명승운

경기대 화학과

Pharmaceutical substances are used extensively in human and veterinary medicine. The drugs that human and animal take are not entirely absorbed by bodies, and are excreted and passed into surface water and treated water. The pharmaceutical substances are having an effect on the environmental pollution and the human body. We established the simultaneous analysis method of macrolide pharmaceuticals (Erythromycin, Tylosin, Virginiamycin and Cimetidine) from treated drinking water. The established method was applied to monitor occurrence of target pharmaceuticals from the treated drinking water in South Korea. Effective sample clean-up and extraction by solid-phase extraction (SPE) prior to LC/MS/MS analysis were performed. Liquid chromatography/tandem mass spectrometry (LC/MS/MS) with electrospray ionization (ESI) was used to the qualification and quantitation of four pharmaceuticals in the multiple reaction monitoring (MRM) mode. The analytes were separated on a Eclipse Plus C18 (2.1×100 mm, 3.5 μm; Waters, U.S.A.) column using a mobile phase of 20 mM ammonium acetate (pH 6.5) and acetonitrile. The established method gave good precision, accuracy, limit of detection (LOD) and limit of quantitation (LOQ). A linear correlation observed in the calibration curves for treated drinking water over the range of 0.005～2.0 ng/mL, showed above r2=0.99. Absolute recovery from treated drinking water was the range of 37.7～106.3%. The limit of detection (LOD) and limit of quantitation (LOQ) for the blank treated drinking water were in the range of 38.7～74.8 pg/mL and 129.0～249.7 pg/mL, respectively. The established method can be used to determine low pg/mL levels of pharmaceuticals substances from the treated drinking water.

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Determination of Hexavalent Chromium in PCB (printed circuit board) and ABS(Acrylonitrile-butadiene-styrene Resin) by Ion Chromatography Coupled with Inductively Coupled Plasma Atomic Emission Spectrometer

김유나, 남상호

목포대 화학과

As in 2006, EU RoHS(Directive on the Restriction of the use of certain Hazardous Substances in electrical and electronic equipment : RoHS) was established. Cr(Ⅵ) is one of the Hazardous Substances. The determination hazardous substance in electronic and electrical products has been very important. Cr(Ⅵ) has been known to have an adverse effect on the lungs, liver, and kidney, RoHS guidelines set a limit of 1000 mg/kg for Cr(Ⅵ) in electrical products. The current method for Cr(Ⅵ) investigated Diphenylcarbazide to complexation with Cr(Ⅵ). Cr(Ⅵ) was finally detected by a UV-VIS Spectrophotometer at a wavelength 540 nm. However, the iron in the sample exists, Diphenylcarbazide react for precipitation the interference the Cr(Ⅵ). Only Cr(Ⅵ) exists in ABS, the NMP(N-Methyl Pyrrolidone) was used for the dissolved of the ABS. The integrity of Cr(Ⅵ) was not changed after alkali digestion of ABS. However, the method was not suitable for the analysis of Cr(Ⅵ) in PCB, Because the iron and cupper in PCB could interference the analysis. In this study, IC was used for the separation of Cr(Ⅵ) in PCB, then was element-selectivity detected by ICP-AES. ABS is one of the polymer that has been widdly used for electrical product. We analyzed Cr(Ⅵ) in ABS, too, by ICP-AES.

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Development of dynamic substrate for selective immobilization of biomolecules

최인성, *김영관, *민달희, 여운석

*건국대 생명공학과 *KAIST 화학과*

Cu(I)-catalyzed Huisgen cycloaddition (click) reaction is widely used for many applications because of its simplicity, mild reaction conditions, high chemoselectivity, and tolerance towards many organic functional groups. Recently, the 'click' reaction has been actively harnessed for immobilization of biomolecules to the surfaces of various materials, particularly self-assembled monolayers (SAMs) on gold. SAMs have been applied to biological studies such as cell adhesion, biochip, and arrays of biomolecules, practically based on the 'static' property of SAMs.In this poster, we report a new surface modification method for affording 'dynamic' property to the surface by activating click reaction on-demand. Our approach utilizes the masked acetylene group, which is not reactive towards click reaction. The acetylene group presented on the surface was blocked by cobalt carbonyl complex. Upon an electrochemical treatment, cobalt carbonyl complex was oxidatively degraded to reveal the acetylene group on the selective region. The resulting acetylene group was used as a chemical handle for surface functionalizations via 'click' with an azide containing molecule. In particular, we designed an azide-modified CGRGDS peptide for cell attachment to the monolayer. As expected, the 'clicked' peptide promoted the selective cell adhesion to the electrochemically induced region. We believe our method can be an important contribution to many applications utilizing click reaction by allowing the 'dynamic' modulation of surface property at the molecular level.

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Liquid chromatographic resolution of various 1-(benzofuran-2-yl)alkanamines on chiral stationary phase (CSP) based on (3,3´-diphenyl-1,1´-binaphthyl)-20-crown-6

박수현, *현명호, *마동희, *정혜정

*부산대 화학 *부산대 화학과*

The benzofuran ring systems feature in a large number of naturally occurring biologically active compounds and in potential synthetic pharmacologic agents. Enantiomerically pure 2-substituted benzofurans might constitute starting materials for the production of biologically active compounds. We had developed liquid chromatographic chiral stationary phase (CSP) based on optically active (3,3´-diphenyl-1,1´-binaphthyl)-20-crown-6 in our laboratory and it has been demonstrated useful for the resolution of racemic compounds with primary amino group.Various 1-(benzofuran-2-yl)alkanamines were prepared and successfully resolved on a CSP based on optically active (3,3´-diphenyl-1,1´-binaphthyl)-20-crown-6. In this study, we will present details for the resolution of 1-(benzofuran-2-yl)alkanamines on the CSP based on optically active (3,3´-diphenyl-1,1´-binaphthyl)-20-crown-6.

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HPLC Resolution of Racemic 1,4-Benzodiazepin-2-ones a CSP based on enantiomeric (3,3'-diphenyl-1,1'-binaphthyl)-20-crown-6

박제영, *현명호, *하진주, *한혜지

*부산대 *부산대 화학과*

Respiratory Syncytial Virus is the cause of one-fifth of all lower respiratory tract infections worldwide and is increasingly being recognized as a serious threat to patient groups with poorly functioning immune systems. 1,4-Benzodiazepine analogues were found to show antiviral activity for respiratory syncytial virus. We successfully resolved racemic 1,4-benzodiazepine analogues which were synthesized in our laboratory on various Pirkle-type CSPs in the previous study. In this study, we have demonstrated that CSP based on enantiomeric (3,3'-diphenyl-1,1'-binaphthyl)-20-crown-6 can be successfully utilized in the resolution of racemic 1,4- benzodiazepin-2-ones.

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A tertiary matrix for analysis of various samples using Matrix-assisted laser desorption/ionization time-of-flight mass spectrometry (MALDI-TOF MS)

홍장미, 신성재, 양효직, 김진희, 이선영, 김정권

충남대 화학과

MALDI-TOF MS (Matrix-assisted laser desorption/ionization time-of-flight mass spectrometry) has been used a powerful tool for analysis of proteomics. Various samples such as proteins, peptides, polyethylene glycol (PEG) and carbohydrates are easily detected using MALDI-TOF MS. The most important thing is that different types of molecules require using of proper matrix to be analyzed. We've been commonly using 2,5-dihydrobenzoic acid (2,5-DHB), but it is well known that α-Cyano-4-hydroxycinnamic acid (CHCA), Sinapic acid (SA) and 2,6-dihydrobenzoic acid (2,6-DHB) are good for analysis of peptides, large molecular proteins and PEG, respectively. Some researchers have studied about a binary matrix which is combination of two matrices. They proved that a binary matrix is superior to a single matrix in some cases due to improved homogeneity of the matrix. In this work, we mixed three matrices (These are DHB, CHCA and SA.) which are most commonly used in MALDI sample preparation. We dissolved 10mg of DHB, CHCA and SA in 1ml of 50% Acetonitrile (ACN)/0.1% Trifluoroacetate (TFA) in water. And this tertiary matrix is mixed with various samples. As a result, it is specially shown that there are high signals for detection of PEG.

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발표종류: 포스터, 발표일시: 금 15:00~17:00

Determination of phenolic compounds change in Paprika varities employing LC-MS/MS

정원영, 김해경, 이정한

경상대 화학과

The fruits of Paprika family are a plentful sources of flavonoids which are known as health benificial secondary metabolites. Paprika(Capsicum annuum var.) is one of the most popular fruits. While the flavonoids of the other paprika fruit are extensively sutdied, researchs for the satsuma have been restricted. In this work, we determined the content and the identies of the flavonoids components using LC-MS/MS.

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Matrix effect on short nucleic acid in the analysis using matrix-assisted laser desorption/ionization time-of-flight mass spectrometry

신성재, 양효직, 김진희, 홍장미, 이선영, 박균하, 박윤봉, 허정석, 김정권

충남대 화학과

Nucleic acids were easily ionized in matrix-assisted laser desorption/ionization time-of-flight mass spectrometry (MALDI-TOF MS) because they have organic bases. Study of nucleic acids is important since nucleic acids contain genetic information. Short nucleic acids were identified in MALDI-TOF MS using different matrices such as 3,5-dimethoxy-4-hydroxycinnamic acid (sinapinic acid, SA), a-cyano-4-hydroxycinnamic acid (CHCA), 2,5-dihydroxybezoic acid (DHB), 3-hydroxypicolinic acid (HPA). We also applied ionic liquid matrix which contains aforementioned matrix with a base such as pyridine or N,N-diisopropylethylamine. Ionic liquid matrix is getting popular as matrix in MALDI-TOF MS since it provides homogeneous mixture of matrix and analyte. Uniqueness of each matrix system will be provided during the presentation.

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Simple Process for Synthesis and Characterization of PEDOT Polymer Coated $LiFePO_4$ Cathode

Hung-Cuong Dinh, *여인형, **조원일, 모선일

*아주대 에너지시스템학부 *동국대 화학과 **KIST 에너지환경연구부*

$LiFePO_4$ is considered to be a promising cathode material for lithium ion battery, due to its low cost, the high theoretical capacity density (170 mAh/g), the excellent reversibility and thermal stability. The application of $LiFePO_4$ is always accompanied with the large cathodical polarization, particularly for high rate demands, because of its low electronic conductivity. Many efforts have been made to improve the electronic conductivity of $LiFePO_4$, including coating conductive carbon, metals or conductive polymer on $LiFePO_4$ surface or doping ions in the crystalline lattice of $LiFePO_4$. In this work, nano-sized LiFePO4 powders are prepared by a hydrothermal reaction from a solution containing LiOH, $FeSO_4.7H_2O$, H_3PO_4, ascorbic acid as reductant and P_{123} as surfactant. The PEDOT polymer can be coated on $LiFePO_4$ surface that increase conductivity of $LiFePO_4$ cathode in the battery. The PEDOT polymer dissolved in a proper solvent to coat the surface of $LiFePO_4$. The characteristics and its performances were investigated by scanning electron microscopy (SEM), X-ray diffraction (XRD), charge-discharge cycle test and cyclic voltammetry (CV) using multichannel battery test mode. The battery characteristics were compared with that of the carbon-coated $LiFePO_4$ cathode.

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Development and application of humic extraction method for less than 100 ml of riverine and/or oceanic water sample

배은정

경북대 화학과

The conventional methods to extract humic material from river or ocean water sample requires at least a couple of liters of sample. This is because of their low extraction efficiency. The typical extraction efficiency is around 30 % and it can be even lower for oceanic water sample. The fact that the methods require a lot of water sample cause a serious analytical problem when only a small amount of sample is available. In this study, a system with electroprep dialysis tank was proposed and tested as the one suitable to extract humic material from a relatively small amount of sample. The humic samples extracted from Youngsan River sample by the proposed system were analyzed by Fourier transform ion cyclotron resonance mass spectrometry for the molecular level identification.

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Analysis of cancer cell phospholipids using positive ion mode high-resolution matrix-assisted laser desorption/ionization Fourier transform ion cyclotron resonance mass spectrometry

양효직, *박규환, **김현식, 김정권

*충남대 화학과 *한국기초과학지원연구원 질량분석개발팀 **한국기초과학지원연구원 질량분석기개발팀*

In this study, we employed a simple method to investigate intact cell lipids using a matrix-assisted laser desorption/ionization 15 T Fourier transform ion cyclotron resonance (FT-ICR) mass spectrometry (MS). Using the advantage of high resolution and accuracy of FT-ICR MS, the unimpaired lipids in acetone was directly analyzed and identified by setting mass tolerance ±1 mDa. Although no MS/MS was performed for the lipids, the exact mass provided almost only one possible chemical composition among possible lipid candidates. In this experiment, positive ion mode was used and the results showed most identified lipids were mainly glycerophospholipids. Using the method, U118 brain cancer cells and human colon cancer cell line HT29 cells were compared with phospholipids profiling.

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The use of Charcoal for Determination of Glycans by Matrix Assisted Laser Desorption Ionization Mass Spectrometry

이선영, 신성재, 양효직, 김진희, 홍장미, 김정권

충남대 화학과

Charcoal adsorbs a wide range of organic compounds dissolved or suspended in gases and liquids. This study describes a method for enrichment of glycans released from chicken ovalbumin using charcoal. To facilitate the glycan analysis, chicken ovalbumin was deglycosylated with PNGaseF for 2hr at 37℃. Charcoal was then applied to remove the remaining proteins. Analysis of the glycans by matrix-assisted laser desorption/ionization mass spectrometer (MADLI-MS) was more effective with 2,6-dihydroxybenzoic acid (2,6-DHB) as matrix than 2,5-dihydroxybenzoic acid (2,5-DHB) as matrix.

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Determination of flavonoid Content change in Citrus unshiu varities employing LC-MS/MS

김해경, 정원영, 이정한, 박세민, 신성철

경상대 화학과

The fruits of citrus family are a plentful sources of flavonoids which are known as health benificial secondary metabolites. Citrus unshiu (satsuma) is one of the most popular fruits. While the flavonols of the other citrus fruit are extensively sutdied, researchs for the satsuma have been restricted. In this work, we determined the content and the identiesof the flavonol components using LC-MS/MS.

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Electrophoretic analysis of sulfonamide antibiotics in a microchip with amperometry

김소진, 원소영, 심윤보

부산대 화학과

A μ-TAS method assembling in-channel preconcentration, separation, and electrochemical detection steps has been developed for sulfonamide antibiotics. An amperometric detection method with a metal oxides modified carbon paste electrode was applied to detect preconcentrated and separated species at the end of the channel. The method was examined for the analysis of five sulfonamide antibiotics of sulfamonomethoxine(SMMX), sulfamerazine(SRZ), sulfadimethoxine(SDM), sulfaquinoxaline(SQX), sulfamethazine(SMZ). Oxidation peaks of them were analyted at 0.9~1.0V, which were selected as an analytical potential for chronoamperometry. Experimental parameters affecting the analytical performance of the method were assessed and optimized.

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Competitive Enzyme Linked Aptamer Assay (cELAA) for dopamine using Avidin-biotin System

박호영, 정소희, 이인숙

서울여대 화학과

Aptamers selected from an in vitro evolution process (SELEX), are short, single-stranded RNA or DNA oligonucleotides that can bind to various targets.Compared with antibodies, aptamers possess plenty of advantages. These have high affinity and specificity, stability, easy synthesis and modification. Thus, aptamers are used as a bio-recognition device instead of antibodies.In this work, a new method for the determination dopamine was developed using competitive Enzyme Linked Aptamer Assay (cELAA). Also, The avidin/biotin system provided amplified signal. Dopamine is an important neurotransmitter molecule of catecholamines. A dose-response curve was constructed, and a limit of detection and dynamic range were accomplished to 3.7×10^{-13} M (8.18 pg/mL) and 1.0×10^{-6} M to 1.0×10^{-10} M, respectively.

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SPR sensing of explosive materials using molecular recognition peptide chips.

양승주, *장성우, 유연규, *박찬량

*국민대 생명나노화학과 *국민대 화학과*

We studied the gas phase detection of the explosives with molecular recognition peptide chip utilizing surface plasmon resonance phenomena. Peptide receptors against explosive materials were screened using phage display technique and immobilized on the gold surface for adsorption of target molecules. The kinetics of adsorption and desorption of the target explosive materials were interpreted by analyzing the time dependent SPR curves. The gas flow system for vaporization of solid compounds was constructed and controlled with MFC. The detection limit of the peptide coated SPR sensor for the explosive was confirmed at several tens of ppb level.

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Analysis of Heavy Metals in Mud and Cosmetics by ICP-OES, ICP-MS, Hg analyzer

나진수, 남상호

목포대 화학과

Mud has been a attractive and potential raw material for cosmetics and shampoo due to the positive effects on skin such as whitening and moisturing. It also has been known that it possibly include the heavy metals such as lead and cadmium. In this study, the various heavy metals in mud and cosmetics has been determined by the several analytical methods. Mercury analyzer was used for the determination of mercury in mud and cosmetics. Cd, Co, Ni, Zn and Mn was determined by ICP-OES and ICP-MS was used for the determination of As and Pb.

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An electrochemical immunoassay based with PVI-Os-HA polymers

박초롱, *최영봉, *김혁한

*단국대 첨단과학부/화학과 *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, and a hydrogel-based electrochemical immunoassay for rapid and quantitative detection of HA. The system employs a conjugate of Osmium (Os) and hippuric acid (HA) and then OS-HA reacts with poly vinyl imidazole (PVI). The competition between hippuric acid (HA) and PVI-Osmium-HA generated electric signals proportional to HA concentration. The electrochemical immunoassay comprised with immobilization of HA-antibody on the nickel-coated ITO electrode and then apply the mixture HA and PVI-Osmium-HA. PVI-Osmium-HA contains hippuric acid-antigen , poly vinyl imidazole (PVI) and 2,2'-Dipyridyl ligand bearing X (X=OCH_3, CH_3). The electrical signal was measured by the voltammetry technique. The resulting currents were linearly related with the concentration of HA complex. Also the structures of Osmium compounds have been identified by the spectroscopic method.

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Simultaneous determination of phoxim and its photo-transformation metabolite residues in eggs using liquid chromatography coupled with electrospray ionization tandem mass spectrometry

Jung Han Lee, Semin Park, Won Young Jeong, Hae-Gyeong Kim, Sung Chul Shin

Department of Chemistry, Gyeongsang National University, Jinju 660-701, S. Korea

A rapid and simple method for determination of phoxim and its photo-transformation compound, phenylglyoxylonitrile thioxime O,O-diethyl phosphorotnate in egg samples of hen and quail is described. Emulsification from the samples was achieved by pretreatment with dehydrating agent, anhydrous magnesium sulfate. Solid phase extraction was performed over silica gel deactivated by 0.5% trimethylamine. Fat was removed from the samples using hexane and extraction was performed with dicholoromethane. Residues were analyzed with a reversed-phase LC-MS/MS using a positive-ion electrospray ionization (ESI) mode. Tebufenozide was used as an internal standard for the quantification of phoxim and its metabolite residues. Identification and quantification of analytes were based on the ion transitions monitored by multiple reaction monitoring (MRM).

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Single Gold Microshell based SERS Probe for Sensitive and Selective Detection of Mercury(II)

한동훈, 임성열, 정택동

서울대 화학부

We have developed a gold microshell-based surface enhanced Raman scattering (SERS) sensor with sensitivity and selectivity for the detection of mercury(II) ions. The gold microshells were synthesized by attachment of Au nanoparticle seed layers to amine-terminated polystyrene beads. This sensor is based on the molecular beacon which involves a Raman-active, tetramethylrhodamine-tagged DNA hairpin structure and provides strategically selective binding of thymine-thymine mismatch for Hg^{2+} ions. The sensor achieved good sensitivity and a limit of detection of 50 nM by monitoring the SERS signal change upon the gold microshell surface-confined Raman reporters. The “signal-on” upon mercury binding could be attributed to a change in conformation from open structure to restricted hairpin structure. The SERS signal showed a linear response with the Hg^{2+} concentration in the range between 50 nM and 1 μM. The selectivity of the sensor was demonstrated by specific discrimination of mercury(II) ion from other various competing divalent metal ions. In addition, a DNA-modified single gold microshell could be individually manipulated using a micropipette. The DNA-modified single gold microshell demonstrated that the determination of mercury(II) ions could be performed successfully in small-volume sample solution (5~10 ㎕).

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Analysis of the Hypochlorous Acid in the Seawater and Laver by Ion Chromatography(IC)

CUI SHENG, 남상호

목포대 화학과

Chlorine in the form of available chlorine has been widely used for the disinfection of public drinking water, waste water and swimming pools. The use of chlorine has aroused much public interest due to adverse effects on aquatic plant and animal life, and also results in the formation of toxic trihalomethanes. The concentration of the available chlorine in the electrolyzed seawater, seawater and laver has been determined by Ion Chromatography in this study. The results have been compared and discussed in terms of the available chlorine.

한국화학회 THE KOREAN CHEMICAL SOCIETY

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Highly sensitive detection of VEGF markers expressed in live cells using aptamer-conjugated nanoprobes

고주희, *추유진, *주재범

*한양대 응용화학과 *한양대 바이오나노공학과*

Angiogenesis, the formation of new vessels, is a highly regulated process. It happens with the process which is complicated in compliance with the interaction of the extracellular matrix substrate. It is known that VEGF is a prominent regulator for both of the physiological and pathological angiogenesis. Thus, VEGF is considered to be a very useful marker for a tumor angiogenesis. In this study, a novel detection method for VEGF protein targets, using aptamer/gold nanoparticle bioconjugates, has been developed. Here, the 5'-terminal of aptamer oliginucleotide was modified with a thiol functional group for a covalent bonding onto the gold surface. In addition, Raman reporter molecules (TAMRA) were covalently bound to the 3'-terminal. When VEGF targets are selectively binding with aptamer conjugated nanoparticles, it induces a conformational change of aptamer molecules. Consequently, the SERS intensities of TAMRA are changed with the concentration of VEGF and this can be used for its quantitative analysis. We demonstrate this conjugation approach to create a imaging probe designed for detection of VEGF, obtaining reflectance images and SERS images of breast cancer cell lines treated with the aptamer-conjugated gold nanoparticles.

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The study of bioethanol purification and quantitative analysis

김태민, 유지선, 한세진, 표동진

강원대 화학과

This study is about the quantitative analysis and the purification process which is a necessary process to produce bioethanol highlighted in the altenative energy field nowadays. In this study, Zeolite is used to raise an ethanol content during distillation process. In order to use bioethanol produced by various biomasses, it comes with the purification process to get high purity. Bioethanol includes water has been analyzed by using special column chromatography device called POLAPACK Q in the quantitative analysis process with Gas chromatography.

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Fast and sensitive trace analysis of formaldehyde using surface enhanced Raman scattering (SERS)-based optofluidic sensor

정은수, 최남현, 주재범

한양대 바이오나노공학과

Formaldehyde is an organic compound used as a building material or a household product but it is known as one of serious environmental pollutants. It is very harmful for human health even at low concentration levels. It also causes irritation of eyes, nose, throat and skin. Therefore, a fast and sensitive detection technique for formaldehyde is needed. Surface-enhanced Raman spectroscopy (SERS) is a well known analytical method that offers great advantages for probing the chemical and structural properties of a compound in microscopic scale. However, it is very difficult to directly perform a quantitative analysis of formaldehyde itself since its SERS signal is very weak. To resolve this problem, formaldehyde was reacted with Schiff's reagent to form alkyl sulfonic acid. This acid shows strong SERS signals and they can be used for the quantitative analysis of formaldehyde. In particular, a SERS-based optofluidic sensor has been used in this work. This method overcomes the drawbacks such as expensive, time-consuming, and complicated sample pretreatment procedures in conventional formaldehyde analysis. We expect, this SERS-based sensor is extensively used in fast and sensitive trace analysis of toxic pollutants in environment.

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A trypsin entrapped poly(diallyldimethylammonium chloride) silica sol-gel microreactor for detecting tryptic peptides of bovine cytochrome c using on-line capillary electrospray ionization mass spectrometry

하지민, 오한빈

서강대 화학과

Proteins entrapped in silicate sol-gel nanoporous are known to generally retain main biological functions, so that they can be used as a biological analysis tool. In the present study, sol-gel entrapped trypsin was used in capillary monolithic column for online digestion followed by electrospray ionization mass spectrometry detection. For this, a fused-silica capillary was coated with poly(diallyldimethylammoniumchloride) (PDDA) through electro-deposition. Then, trypsin-entrapped sol-gel material was inserted into the prepared capillary. For cytochrome c, we could detect cytochrome c peptides in ESI-MS spectra. In the poster, further experimental details will be presented.

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Studies on the Biological Activities of *Lycoris squamigera*

김보미, *남선미, *채규윤

*원광대 생명나노 화학과 *원광대 화학과*

Lycoris squamigera (resurrection lily) is a plant in the amaryllis family, Amaryllidaceae.In this study, antioxidant and antibacterial, anti-inflammatory effect of *Lycoris squamigera* methanol extract and different solvent fraction was carried out. *Lycoris squamigera* was extracted with methanol (80% methanol) and then proceeded solvent extraction with n-hexane, ethyl acetate (EA), and butanol (BuOH). Crude extract and solvent fractions along with control standards were measured for their anti-oxidative activity using three different methods; free radical scavenging activity (DPPH), reductive potential test, and total phenolic content. The anti-oxidative activity of the fractions was measured and compared with control such as butylated hydroxyanisole (BHA), butylated hydroxytoluene (BHT), and α-tocopherol. The antibacterial activity of samples were evaluated by MIC test. The nitric oxide (NO) production was measured by Griess reagent system and preformed to MTT assay. The MTT assay was showed a quantification of viable cells that was dyed by metabolic activity cell. Key words: *Lycoris squamigera*, Antibacterial activity, Anti-oxidative activity. Anti-inflammatory effect

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Surface-enhanced Raman scattering in nanoliter droplets:towards high-sensitivity detection of mercury (II) ions using aptamer-conjugated nanoparticles

황선영, Han Xiao, *이상엽, *고주희, 주재범

*한양대 바이오나노공학과 *한양대 응용화학과*

Simple and sensitive aptamer-based surface-enhanced Raman scattering (SERS) detection of mercury ions (Hg2+) using gold nanoparticles (AuNPs) has been developed. It is based on the fact that AuNPs interact with single-strand DNA. The anti-Hg2+ aptamer is rich in thymine (T) and readily forms T–Hg2+–T configuration in the presence of Hg2+. As SERS is a promising alternative for high-sensitivity analysis of mercury (II) ions, when small fluorescent molecules are adsorbed on AuNPs, their SERS signals are strongly increased. But, when in the presence of mercury (II) ions, a proportion of these molecules are released from the metal surface causing a decrease in the observed SERS signal.The approach of droplet-based microfluidics combined with SERS detection provides both fast and sensitive detection of Hg2+ in water. Manipulation of such droplets through winding microchannels affords rapid and efficient mixing of the contents. Quantitative analysis of Hg2+ was performed by calculating spectral raman peak area of TAMRA at 1,651 cm−1. The proposed analytical method offers a rapid and reproducible trace detection capability for Hg2+ in water.

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Microfluidic chip-based electrochemical oxygen sensor

전원용, 최영봉, 김혁한

단국대 화학과

The quantitative determination of oxygen in atmospheres and waters is very important for environmental, process control and safety reasons. There are several types of electrochemical sensors. An electrochemical oxygen sensor using a printed glassy carbon electrode for continuous monitoring of oxygen has been developed which apply a wide range of industry. We have been detected the dissolved oxygen (DO) using an electrochemical sensor with the electrodeposited the Pt nano-particles onto the screen printed carbon electrodes (SPCEs). The electrical signals were measured by the voltammetric technique. The resulting currents were linearly related with the concentration of oxygen through the i-t curve. A study of the electrochemical oxygen sensor offer the cheap, portable devices of detecting for continuous dissoved oxygen (DO) concentration.

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Sol-gel derived multiwalled carbon nanotube-thiol substituted silica /gold nanoparticles composites – A robust matrix for enzyme immobilization and electrochemical determination of ionic pollutants

이광필, *A.Gopalan, **Shanmuga sundaram Komathi

*경북대 화학교육과, NANOKGM *경북대 화학과, NANOKGM **경북대 화학과*

The multiwalled carbon nanotube (MWNT) /thiol substituted silica (Si(SH)) composite was prepared by sol-gel technique. Si(SH) unis were covalently linked MWNT through insitu complex hydroxylation/condensation process. Subsequently, gold nanoparticles (Au NPs) were electrodeposited onto MWNT/Si(SH) matrix. The morphology of MWNT-Si(SH)/ AuNP composite was examined using field emission scanning electron microscopy. The amount of Au NPs and lattice structures were determined through EDAX and x-ray diffraction (XRD) measurements. Cytochrome c (cyt c) was drop casted onto the surface of MWNT-Si(SH)/ AuNP. The electrochemical characteristics of MWNT-(S)-SH/GNPs/cyt c electrodes were evaluated by cyclic voltammetry and electrochemical impedance spectroscopy. The of MWNT-(S)-SH/GNPs/cyt c electrodes were used for the electrochemical determination of nitrite ions.

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Evaluation of antioxidant activity and active aubstances analysis via stepwise separation of water-soluble extracts from Korean black pine(Pinus thunbergii) bark

신장철, *주성진, *김일광

*원광대 화학과 *원광대 생명나노화학부*

Antioxidant activities and substances analysis follow with stepwise separation were investigated to identify an effective substances and to compare variation of antioxidant activities between a single substance and mixture in crude extract the water extracts Korean black pine bark (Pinus thunbergii) were separated by column chromatography in order of solvent polarity and HPLC of gradient solvent system. Antioxidant activities of solvent extracts and fractions of stepwise separation were measured with various assays including free radical scavenging activity, reductive potential, and total phenolics content. The toxicity (cell viability) of water crude extract was examined by MTT test and the fractions of stronger antioxidant activities were analyzed to find active substances by TLC, HPLC-mass sepectrometry, ^{1}H-NMR, and ^{13}C-NMR

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Analysis of Low Frequency Raman Specrta of L-cystine

강원석, 김효섭, 강신범, 김재호

아주대 분자과학기술학과

Low-frequency Raman spectroscopy provides information on local structure of solutions coupled with hindered translational and librational motions. Raman spectra for L-cystine in the translational vibration region have been studied extensively by many groups. L-cystine has been studied using low frequency Raman spectroscopy. In the Raman scattering experiment, the light source of 514.5 nm from a Ar ion laser was utilized with an output of 500 mW. The scattered light from the specimen was analyzed by a triple monochromator. We report low frequency Stokes Raman spectra in the range between 70 and 200 cm-1

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Electrodeposition of Nanodiamond/polyaniline/gold nanoparticles composite and fabrication of cytochrome c immobilized biosensor

A.Gopalan, *이광필, **Shanmuga sundaram Komathi

*경북대 화학과, NANOKGM *경북대 화학교육과, NANOKGM **경북대 화학과*

Polyaniline incorporated nanodiamond (PANI/ND) was electrodeposited onto the surface of indium tin oxide coated glass electrode (ITO) by cyclicvoltammetry through electrochemical polymerization of aniline in the presence of functionalized ND. Further, gold nanoparticles (AuNPs) were embedded into PANI/ND film by constant potential electrolysis of gold(III)chloride solution. Finally, cytochrome c was immobilized onto the surface of PANI/ND/Au NP to obtain the biosensor, PANI-g-ND/AuNPs/cyt c. The morphology changes in the electrode modification process was investigated using field emission scanning electron microscopy. The amount of AuNPs incorporated into the electrode was estimated by x-ray photoelectron spectroscopy (XPS). The electrochemical properties of the PANI-g-ND/AuNPs/cyt c were studied systematically, using cyclic voltammetry (CV) and electrochemical impedance spectroscopy (EIS) measurements. The biosensor electrodes were utilized for the selective determination of nitrite ions.

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Discussed the anti-oxidative and anti-inflammation effects of the flavonoids compound isolated from the Acer Palmatum Var amoenum leaves

신장철, *주성진, *김일광

*원광대 화학과 *원광대 생명나노화학부*

he Acer Palmatum Var amoenum leaves were extracted with methanol at room temperature and the extracts were separated to five partitions by hexane, chloroform, ethyl acetate, butanol and water. The yield of the parts were determined with percentage and some flavonoids compound as vitexin and quercetin-3-o-glucoside were isolated by silica gel and Sephadex LH-20 chromatographic method, the anti-oxidative and anti-inflammation effect evaluated by DPPH radical scavenging assay; total phenolics method; and inhibited nitric oxide test, and the standard BHA, BHT, α-Tocopherol were used in antioxidant ability evaluation.

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Quantitative analysis of paraquat herbicide using surface-enhanced Raman scattering-based optofluidic sensor

Rongke Gao, *Huang Jjianshe, **최남현, **주재범

*한양대 응용화학과 *한양대 바이오나노산업기술인력양성사업단 **한양대 바이오나노공학과*

Paraquat (PQ) is a highly effective contact herbicide that is worldwidely marketed as a fast-acting, non-selective compound for broadleaf weed control. Compared with most pesticides, however, PQ is extremely toxic to humans and the lack of strategies to manage PQ poisoning has resulted in high fatality rates. A number of analytical methods, including high-performance liquid chromatography (HPLC), gas chromatography mass spectroscopy (GC-MS), Voltammetric, and time-resolved fluoroimmunoassay (TR-FIA) methods, have been reported. In this work, a rapid and highly sensitive trace analysis of PQ using surface-enhanced Raman scattering (SERS)-based optofluidic sensor has been developed. Here, microdroplet channel has been fabricated for its quantitative analysis. Under the optimal condition of flow velocity, PQ molecules were effectively adsorbed onto silver nanoparticles in the channel. A quantitative analysis of MG was performed based on the characteristic peak height in its SERS spectrum. Here, we introduce a new conceptual detection technology, using a SERS optofluidic sensor, for the highly sensitive trace analysis of PQ in water.

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Free radical initiated peptide sequencing II

이윤진, 문봉진, 오한빈

서강대 화학과

TEMPO-FRIPS method is previously shown to be another complementary tandem mass spectrometry tool useful for peptide sequencing. In TEMPO-FRIPS, a TEMPO radical initiator is often attached to an undesired place as well as to a desired N-terminus, which often hampers peptide sequencing. To overcome this drawback, a new approach is sought. Initially, undesired places are masked and then a TEMPO initiator is attached to the N-terminus. The peptides prepared in this way were further subjected to tandem mass spectrometry. In this poster, we will show the detailed experimental procedure and results for this new approach.

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Electrochemical synthesis of lithium trivanadate/polypyrrole (LiV_3O_8/PPy) composite film as a cathode

Quang-thao Ta, *여인형, **조원일, 모선일

*아주대 에너지시스템학부 *동국대 화학과 **KIST 에너지환경연구부*

Lithium trivanadate, LiV_3O_8, is an attractive electrode material for lithium ion batteries due to its structural flexibility with Li^+ insertion, high specific capacity and long cycle life. Nanostructured LiV_3O_8 was prepared by controlling the solution pH, the nucleation processes and annealing temperature. The electrical conductivity of the electrodes composed of nanosized inorganic materials can be increased by making composite with conducting polymers. The conducting polymer acts as a conducting matrix, a binder and an active material as well as volume change buffer agent. In this work, thin films of lithium trivanadate/polypyrrole (LiV_3O_8/PPy) composite, suitable for lithium ion battery cathodes, were successfully synthesized by an electrochemical method. The structural, compositional and morphological analysis of the XRD patterns, FTIR spectra and SEM image show that the polypyrrole were electrochemically grown to make the uniform composites with the dispersed LiV_3O_8 which could significantly enhance the electrical conductivity and stability of the composite electrode. Electrochemical measurements also reveal that LiV_3O_8/PPy composite exhibits a good reversibility, higher stability and better cycle life than the electrodes made of LiV_3O_8 only.

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Polydimethylsiloxane Mini-Disk Extraction for the Analysis of volatile fragrance compounds from lemon and orange essential oils by GC/MS

장혜진, 이동선

서울여대 화학과

The aim of this study is to application of a novel sampling method called headspace polydimethyl-siloxane (PDMS) mini-disk extraction (HS-PDE) combined with GC/MS for the analysis of flavor compounds from lemon and orange essential oils. Major flavor compounds of lemon and orange essential oils are limonene, sabinene. In this study, we compare two different sampling methods. The HS-PDE was compared with headspace solid phase microextraction (HS-SPME). The flavor composition of lemon and orange essential oils by two different sampling methods is qualitatively and quantitatively similar. Additionally, comparing the CF(concentration factor) values as relative extraction efficiency by HS-PDE and HS-SPME. HS-PDE and GC/MS is a very promising sampling technique for the characterization of flavor compounds from liquid essential oils.

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Supercritical Fluid Extraction of Phytoncide from *Pinus koraiensis* leafs.

유지선, 표동진

강원대 화학과

The composition of phytoncide extracted from *Pinus koraiensis* leafs growing wild in Korea(Whachoen) was studied by Supercritical carbon dioxide extraction. Extraction efficiencies under several different extraction conditions were examined. For SFE, pressure, temperautre, organic modifier content, were examined. The analysis of the extracts were performed by GC/MSD. The major constituents in extracts of *Pinus koraiensis* were sesquiterpene as δ-cadinene, γ-MuuroleneGermacrene-D, β-caryophyllene and bicyclic monoterpene as trans bornyl acetate.

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Preparation and characterization of novel polymer network hydrogel microspheres consisting of gold nanostructures

김민경, A.Gopalan, *이광필

*경북대 화학과 *경북대 화학교육과*

New kind of polymer network hydrogel microspheres has including gold nanostructures (PNHG-Au) has been developed. PNHG-Au consists of two polymers crosslinked into a network and incorporated with Au nanostructures. The proportions of the polymers in the network are independently varied. Fourier transform infrared spectroscopy (FTIR) was used to analyze the structural characteristics of PNHG-Au. Lower critical solution temperature (LCST) and glass transition temperature (Tg) of PNHG-Au were determined from differential scanning calorimetry measurements. The equilibrium swelling ratio of PNHG-Au was obtained as a function of pH and temperature. The drug releasing capacity and the release kinetics of PNHG-Au were evaluated using a model drug.

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Preparation of novel sulfonated poly(ether ether ketone)- conducting polymer composites for direct methanol fuel cells

이세희, *M. Francklin Philips, **A.Gopalan, ***이광필

*경북대 나노과학기술과 *경북대 차세대에너지기술연구소 **경북대 화학과 ***경북대 화학교육과, 경북대 나노과학기술과*

Direct methanol fuel cells (DMFCs) using proton conductive polymer electrolyte membranes (PEMs) as one of the key components are promising future power devices in automotive, stationary and portable electronic applications. One of the problems in DMFCs is the methanol cross over through the membrane. In the present work, in order to make methanol-blocking layer to reduce the methanol crossover, new polymer electrolytes, sulfonated poly(ether ether ketone) (SPEEK)/conducting polymer blends were prepared. Blend membranes were prepared with various weight ratios of SPEEK to conducting polymer. The blends were characterized by X- ray diffraction, Fourier transform infrared spectroscopy, thermogravimetric analysis and differential scanning calorimetry. The surface morphology was determined by field emission scanning electron microscopy. Physico-chemical characteristics such as water and methanol uptake behavior, methanol permeability, ionic exchange capacity and proton conductivity of the blend membranes were determined. The proton conductivity of the blend membranes was measured by impedance spectroscopy at different temperatures. The proton conductivity of the blend membranes was found to increase with increasing content of conducting polymer in the blends as well with temperature. The DMFC performance using the blend membrane was evaluated.

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Investigation of sulfonated poly(ether ether ketone based new composite membranes for moderate temperature fuel cell application

이세희, *M. Francklin Philips, **A.Gopalan, ***이광필

*경북대 나노과학기술과 *경북대 차세대에너지기술연구소 **경북대 화학과 ***경북대 화학교육과*

Recently, poly(ether ether ketone) (PEEK) has been proved to be a promising membrane material for fuel cell applications because of its lower preparation cost, good film forming properties, and also chemical, thermal and mechanical stability. However, scientists are continuously working on improving the performance characteristics of PEEK based membranes. In this work, We report the preparation of sulfonated poly(ether ether ketone) (SPEEK)–silica –conducting polymer composite membranes and their use in direct methanol fuel cells (DMFCs). Silica was incorporated into the SPEEK membrane by sol–gel method. SPEEK–silica membranes surfaces were insitu loaded with a conducting polymer. A systematic investigation of the composite membrane in terms of physico-chemical properties such as water and methanol up take studies and ionic exchange capacity, methanol permeability and proton conductivity reveals the usefulness in DMFCs. The composite membranes were characterized by 1H NMR, FTIR, XRD and TGA. The proton conductivity of the composite membrane was obtained by AC impedance spectroscopy. Owing to the adequate proton conductivity, reduced methanol permeability, convenient processability and low cost, the new composite membranes could be considered as the alternative membranes for moderate temperature DMFCs.

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Rapid and highly sensitive detection of noxious materials using SERS-based alternative micro-droplet generator

최남현, 추유진, 이문권, 주재범

한양대 바이오나노공학과

Recently, We have developed a surface-enhanced Raman scattering (SERS)-based droplet platform for a rapid and highly sensitive detection of chemical, environmental and biological analytes. Droplet-based microfluidic systems have gained increasing popularity in recent years. Such systems allow the generation and manipulation of monodisperse nanoliter sized liquid droplets within an immiscible carrier fluid in a high-throughput manner. Compared to single phase flow, the localization of reagents within discrete and encapsulated droplets enhances mixing, minimizes residence time distributions, and affords ultrahigh analytical throughput. However, to become a core instrumental platform, high-sensitivity online droplet detection remains a significant challenge. Herein, we demonstrate the use of SERS detection technique for the highly sensitive trace analysis of noxious materials in water within a droplet-based microfluidic system.

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Multifunctional electrospun nanowebs incorporated with carbon nanotubes-gold nanoclusters

김태경, *A.Gopalan, **이광필

*경북대 나노과학기술학과 *경북대 화학과 **경북대 화학교육과, 경북대 나노과학기술학과*

The incorporation of metal nanoparticles and carbon nanotubes into polymer nanofibers can produce functional nanofibers having optical, electrical, or biocatalytic properties. Electrospinning was employed to prepare new multi-functional nanowebs. Cyclodextrin based inclusion complex (CD-IC) was used to disperse multiwalled carbon nanotubes (MWNT) into the electrospun polyvinylidene fluoride (PVdF) nanofibers and the composite nnaofibers, MWNT(CD-IC)/PVdF-NFMs, were obtained. Then, MWNT(CD-IC)/PVdF-NFM was loaded with gold (Au) nanoparticles. The structure and morphology of Au/MWNT(CD-IC)/PVdF-NFM were investigated by transmission electron microscopy (TEM), field emission scanning electron microscopy (FE-SEM), FT-IR spectroscopy, X-ray diffraction spectroscopy (XRD), thermogravimetric analysis (TGA) and differential scanning colorimetry (DSC). The new Au/MWNT(CD-IC)/PVdF-NFM exhibits excellent electrocatalytic activity towards oxidation of ascorbic acid.

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Metal nanoparticles anchored new multiwall nanotubes based composites as electrocatalysts

이현규, *A.Gopalan, **이광필

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The uniform distribution of electrocatalytically active metal nanoparticles (MNPs) and metal oxide nanoparticles (MONPs) onto the surface of multi walled carbon nanotube (MWNT) is important for the preparation of highly efficient electrode materials for fuel cell applications. In the present work, we report the preparation of new composites based on MWNT with uniform dispersion of MNPs and MONPs onto its surface. The MWNT/MONP/MNP composites were characterized for morphology, structural and other physic chemical characteristics by field emission scanning electron microscopy, UV-visible spectroscopy, Fourier transform infrared spectroscopy, Raman spectroscopy, x-ray diffraction measurements. The electrocatalytic activities of the new composites were tested for oxidation of methanol.

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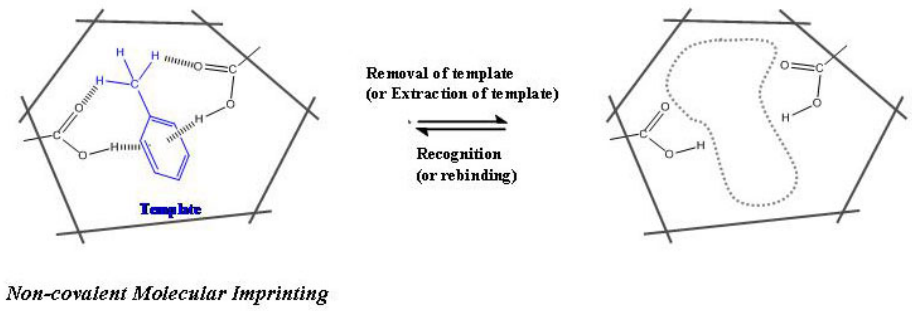
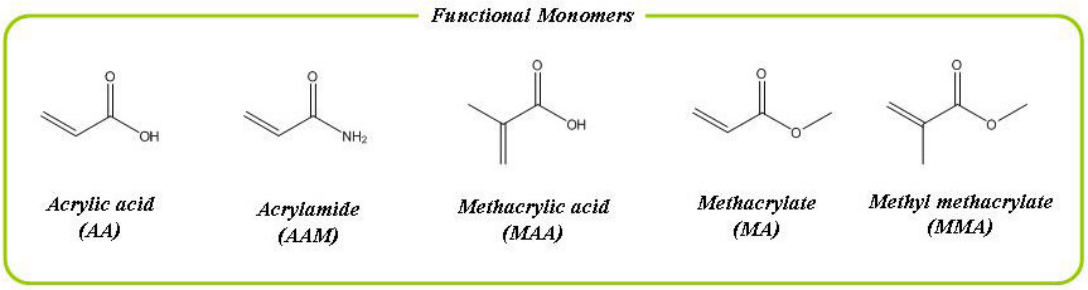
SPR study on the sensing of gaseous toluene utilizing molecularly imprinted polymer films

장성우, *임상규, *유연규, 박찬량

*국민대 화학과 *국민대 생명나노화학과*

We applied molecularly imprinted polymer films to the sensing of gaseous formaldehyde and toluene using SPR technique. The molecularly imprinted polymer films of SPR chip for the sensing of toluene were synthesized by UV induced polymerization method using several functional monomers and the morphology of polymer films were obtained by atomic force microscopy at various thicknesses. The sensitivity and selectivity were compared with non-imprinted polymer films.





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Nanodiamond based conducting nanomeshes : One step synthesis and electrochemical application

Shanmuga sundaram Komathi, A.Gopalan, *이광필

*경북대 화학과 *경북대 화학교육과*

Nanodiamond (ND) based conducting nanomeshes were prepared through one-step enzymatic polymerization process. The nanomesh was prepared with a mixture of ND, aniline and a cross linker. The enzyme induces the formation of conducting mesh and simultaneously be entrapped to result ND/PANI/HRP-NM. The morphology of ND/PANI/enzyme-NM. Field emission scanning electron microscope was used to investigate the morphology. The electronic state was determined by UV-visible spectroscopy The electrochemical characteristics of ND/PANI/HRP-NBM thin film was evaluated and the electron transduction capability between the enzyme and electrode was analyzed. The nanomesh shows the characteristics of establishing direct electrochemistry and usefulness as a matrix for electrochemical determination of biomolecules.

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Preparation of novel substituted polyaniline/ gold nanoparticles nanostructures using porous template.

Shanmuga sundaram Komathi, *S. Palaniappan, *P. Manisankar, A.Gopalan, **이광필

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It is known that the properties of metal nanostructures can be tuned by varying the parameters such as their size, structures and morphology. Significant progress has been made in fabricating simple nanostructures such as nanowires and nanotubes over the past few years However, the fabrication of multifunctional nanodevices requires more dimensional complex nanostructures. In this work, we report the preparation of gold nanoparticles (AuNPs) anchored substituted polyaniline (PANI-S) nanostructures using anodisc alumina (AAO) as the basal template. Substituted aniline molecules were self aligned in the pores of AAO in the presence a surfactant. Self-alligned substituted aniline moieties were polymerized using oxidative polymerization. Finally AuNPs were anchored to to obtain PANI-S/AuNPs-NS. The morphology and the other physico chemical characteristics of the prepared PANI-S/AuNPs-NS were examined through field emission scanning electron microscopy (FESEM), UV-visible spectroscopy , Fourier transform infrared spectroscopy , x-ray diffraction and thermogravimetric analysis . The electrochemical behavior of PANI-S/AuNPs-NS composites was determined through cyclic voltammetry and electrochemical impedance spectroscopy measurements.

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Insitu formation of poly (4- Amino diphenyl amine) / silver nanoparticles composites in p-toluene sulphonic acid medium : A kinetic analysis using UV- Visible spectroscopy

M. Francklin Philips, *Starlet Thanjam, M. Francklin Philips, **Shanmuga sundaram Komathi, *P. Manisankar, ***C.Sivakumar, **A.Gopalan, ****이광필

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Chemical oxidative polymerization has been used to insitu generate poly (amino diphenyl amine/ silver nanoparticles composites (PADPA-Ag NPs composite). UV-vis spectroscopic method was used for following the course of polymerization of 4-aminodiphenyl amine using silver nitrate as the oxidant in p-toluene sulphonic acid medium. Kinetic studies were performed by monitoring the absorption spectra of the reaction medium at different conditions. Rate of polymerization (Rp) was determined under different conditions. The PADPA-Ag NPs composite was separated from the reaction medium The amount of PADPA-Ag NPs composite was estimated for different time intervals during the course of polymerization. A kinetic equation was established relating the Rp with [ADPA] and [oxidant]. The rate constant for the formation of PADPA-Ag NPs was deduced. The dependences of Rp on the experimental conditions were used to arrive at a rate expression for the for the formation of PADPA-Ag NPs nanocomposite.

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SPME fiber와 Depletion 추출법을 이용한 BTEX의 분배계수의 결정 방법

엄인용

대구가톨릭대 생명화학과

Solid Phase Microextractin (SPME) Technique 은 비교적 근래 (1990 년대)에 개발된 sampling/sample preparation 방법으로 현재 여러 가지 시료 특히, water sample 로부터 다양한 물질들 (약품, 농약, BTEX, 등)의 농축을 손쉽고 빠르게 수행할 수 있는 장점이 있다. 전통적으로 SPME fiber 를 이용한 여러 가지 화합물의 분석법 개발이 많은 연구자들에 의해 주목을 받고 있지만, 수용액에서 유기화합물이 SPME fiber 에 얇게 코팅되어 있는 비극성 유기층, polydimethly siloxane (PDMS)에 농축되어 평형(equilibration)에 이르게 되면 화합물이 물과 fiber 사이에 분배되는 원리를 이용하여 수용액 내에 포함된 여러 유기화합물(organic compounds)의 분배계수 (partition coefficient) 결정에도 활용될 수 있다. 분배계수는 보통 shake-flask 방법에 의해 결정하여 왔는데 이 방법은 단조로운 작업과 여러 가지 과정을 통해 시료가 유실될 수 있수 있으며 특히 시간이 오래 걸린다. 이에 반해 SPME fiber 를 활용한 분배계수의 결정은 보다 쉽고 빠르게 수행 할 수 있다는 장점이 있다. 기존의 발표된 SPME fiber 를 활용한 분배계수 결정법은 대상 화합물의 수용액에서의 일련의 표준용액을 사용해야만 한다. 또한 fiber 에 의해 추출된 화합물의 양을 매우 정밀하고 정확하게 측정해야만 정확한 분배계수를 정확하게 구할 수 있다. 반면에 multiple extraction approach (depletion method)를 이용한 분배계수 결정법은 한 가지 농도의 표준용액만 필요하고 (혹은 화합물의 초기 농도를 모르더라도) 연속적인 추출 (consecutive extraction or depletion extraction)에 따른 분석장비의 상대적인 signal 크기의 비를 이용하여 유기 화합물의 분배계수를 결정할 수 있는 장점이 있다.본 연구에서는 SPME fiber (PDMS)와 depletion method 를 이용하여 benzene, toluene, ethylbenzene, xylene (BTEX)의 분배계수를 구하였다. Data analysis 는 Excel Solver 를 이용하였고 분배계수의 log 값(logK)은 2.39 (benzene), 2.70 (toluene),

2.85 (ethylbenzene), 2.96 (p-xylene)로 문헌치와 큰 차이가 없음을 확인하여 본 접근법이 유용함을 입증하였다. 이 방법은 emerging contaminant 와 같은 새로운 오염원의 분배계수를 결정하는데 유용하게 쓰일 수 있을 것이다.

대 한 화 학 회
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Determination of trace bromate in drinking and mineral water by direct-injection ion chromatography with triiodide post-column method

고희정, 신승희, 강창희, *김정례

*제주대 화학과 *(주)제이엘사이언스*

Bromate (BrO_3^-) is a disinfection by-product formed during the ozonation of bromide-containing mineral and drinking water. The World Health Organization (WHO) classified bromate as possible human carcinogen for which reason most countries stipulate bromate limits between 10 ug/L. The US Environmental Protection Agency (US EPA), the European Union (EU) and Korean government currently prescribe a maximum bromate concentration of 10ug/L. In this study, trace level bromate has been determined according to US EPA 326.0. The method was based on the triiodide formation during post-column derivatization, in order to reduces any bromate in the sample to bromide under the catalytic influence of ammonium heptamolybdate at room temperature. The triiodide produced in pcr reaction was detected by UV at 352 nm. From the experimental results, bromate was determined below 0.5 ~ 5.0 ppb level. The method detection limit was 0.16 μg/L by 7 injection of 3 μg/L certified bromate standard.

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Different UV absorption spectra between R- and S- enantiomers

shabiabbas, 정원조

인하대 화학과

In this study, appearance of enantiomer peaks of unequal peak areas in chiral separation as well as different UV absorption spectra of the enantiomers are presented. It is generally known that the R- and S-enantiomers have the same physical properties including UV absorption. Suspicion of different UV absorption spectra between a pair of enantiomers was occurred when the chromatograms of some enantiomers were examined in MIP-LC and MIP-CEC study. We have observed different UV absorption spectra between R- and S- enantiomers in the solvent system composed of acetate buffer and acetonitrile for two pairs of enantiomers--- ketoprofen and flurbiprofen. Presumably, this phenomenon may be caused by formation of different analyte- solvent complexes between R- and S- enantiomers. Workers in chiral separation study are alerted to similar happenings.

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Effects of protein adsorption on the colloidal properties of sub-100 nm sized P25 TiO2 dispersions

이송희, 권동욱, 윤태현

한양대 화학과

Despite of the widespread use of manufactured nanomaterials (MNs) in many industrial applications and consumer products, only limited information is available on their potential risk on the environments and human health. Here, the effects of protein adsorption on the colloidal properties of P25 TiO2 (P25, Evonik/Degussa GmbH) dispersion were investigated. Especially, adsorption properties of bovine serum albumin (BSA) proteins on sub-100 nm fraction of P25 TiO2 , such as Kads and Γmax at pH7.0, were carefully measured and their agglomeration and sedimentation kinetics in in vitro cytotoxicity test media (i.e., RPMI-1640 and DMEM) were carefully studied. We found that the added concentrations of proteins play an important role in stabilizing TiO2 particles in cell culture media. As a result of this study, optimum preparation protocols for preparing stable TiO2 nanoparticle dispersions with well-defined particle size distributions were found, which can be used as a part of standard MN test guidelines for producing more reliable, reproducible and impartial in vitro toxicity test results of MNs.

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Development of Oyster certified reference material for accurate measurement of arsenobetaine based on the isotope-dilution LC-MS/MS

이우영, *이경석, *임용현, *임영란, 김태규, *황의진

*부산대 화학과 *한국표준과학연구원 분석화학표준센터*

Determination of arsenic in marine organisms have extensively studied that a plenty of arsenic-containing compounds are identified and represented to different level of toxicity depend on their chemical forms. However, organo-arsenic species (e.g. AsB) show lower toxicity rather than inorganic species so that only the measurement of total content of arsenic can mislead into overestimation of toxicity of arsenic in food safety. In this study, we have focused on the development of oyster certified reference material (CRM) for accurate measurement of arsenobetaine, which is the one of the major arsenic species in seafood. The isotope-dilution LC-MS/MS method for the analysis of arsenobetaine has been developed to assign the certified value and various sample preparation method such as ultrasonication and microwave-assisted extraction were also tested for method validation. The measured values through the different sample preparation method show good agreement and the Oyster CRM shows good homogeneity.

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Preparation and Characterization of Stable Nano-Silver Dispersions for Nanotoxicological Studies.

박재홍, 권동욱, 윤태현

한양대 화학과

With mass production and global use of manufactured nanoparticles (NPs), such as nano silver (nano-Ag), concerns about the potential risk of nanoparticles to the environment and human health are increasing. However, despite of their importance, only limited information is available on the behavior of their colloidal suspensions (e.g., agglomeration, aggregation and precipitation) in the media. In this study, we investigated the effects of concentrations of stabilizer such as citrate on the colloidal stability of nano-Ag in moderately hard water (MHW), commonly-used medium for ecotoxicological test, by measuring optical density and hydrodynamic size tried to induce the optimum ratio between nano-Ag and citrate for maintenance of stable colloidal suspension. In the same manner, the effect of growth supplement such as fetal bovine serum (FBS) in RPMI1640 cell culture medium was also examined. TEM micrographs showed that nano-Ag particles prepared with the deionized water were spherically shaped and composed of particles with sizes less than 15 nm. The agglomeration rate and sedimentation rate decreased as the concentration of citrate or FBS added increased. Nano-Ag suspensions (12.5 mg/L) in the MHW containing 2.50 mM citrate or in the RPMI1640 containing 10 % FBS showed higher stability up to 72 h and 36 h, respectively. The size of the agglomerates was significantly reduced when citrate concentration in the MHW increased from 0.25 to 2.50 mM and when FBS concentration in the RPMI1640 increased from 0.01 to 10%, respectively. From the result of this study, we derived an optimum condition for preparation. For MHW media, 2.50 mM citrate ion were required to maintain colloidal stability of nano-Ag and for RPMI1640 media, 10% FBS were required.

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Development of tomato paste certified reference material for the accurate measurement of Tin, Lead and Cadmium in canned foods

조항미, 이경석, 임용현, 임영란, 황의진

한국표준과학연구원 분석화학표준센터

식품 중의 무기원소의 정확한 측정은 식품안전과 환경의 측면에서 항상 매우 중요한 이슈가 되어왔고, 측정의 정확성과 신뢰도를 올리기 위해서는 믿을만한 인증표준물질의 사용이 필수적이다. 이 연구에서는 통조림의 형태로 보관되는 식품 중 주석과 카드뮴, 납의 측정을 위한 인증표준물질의 개발과 인증방법에 관해 소개하고자 한다. 주석은 식품의 장기보관을 위한 통조림 내부의 강철판의 부식을 방지하기 위해 많이 사용되고 있으며 보관하는 동안 식품 속으로 조금씩 용출된다. 특히 토마토와 같은 산성식품의 경우에는 주석의 용출이 더욱 빨라질 수 있으며 한국식품의약품안전청(KFDA)에서도 통조림 식품 중 주석의 농도수준을 최소화하기 위해서 우수제조규범에 따라 제조하도록 지도하고 있다. 따라서 식품 중 주석 및 다른 유해원소 측정의 신뢰성과 소급성을 제공하기 위해서 토마토 페이스트 인증표준물질의 개발을 수행하였다. 토마토 페이스트 인증표준물질은 균질성 확보와 오염을 방지하기 위해 통조림에 보관된 원료물질로부터 잘 관리된 환경에서 제조되었고, 최상위분석법인 동위원소희석질량분석법에 기반한 ICP-MS 법을 적용하여 인증값을 부여하였다.

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Development of Double Resonance Solid-state NMR Probe for the Structural Studies of Membrane Proteins

박태준, 엄승훈, 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. Solid-state NMR experiments on lipid bilayers or bicelle samples are valuable for membrane proteins with a predominantly helical secondary structure. Because these oriented samples takes advantages of the spectral simplifications that result from uniaxial orientation parallel to the direction of applied magnetic field. Especially, the sample preparation of the bicelles is easier and the bicelle samples are more stable than mechanically oriented lipid bilayer samples between glass plates, so that they can be kept for more than a year. So magnetically aligned bicelle samples in recent years are frequently used to determine the structure of membrane proteins by solid-state NMR spectroscopy. In this study, the double resonance probe has been designed to carry out polarization inversion spin exchange at the magic angle (PISEMA) or SAMMY experiments to obtain orientational constraints for the aligned membrane proteins in lipid bicelle environment at 400MHz wide-bore magnet. Here, we present the construction of home-built solid-state NMR probe and the 1H-15N 2D SAMMY spectra of crystal and bicelle samples.

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Colloidal properties of sub-100 nm P25 TiO_2 in reconstituted freshwater media for nanotoxicity testing under UV exposure conditions

권동욱, 이송희, 윤태현

한양대 화학과

Mass production and widespread use of manufactured nanomaterials, such as nanosized titanium dioxide (nano-TiO_2), in industrial applications and consumer products have raised increasing concerns regarding the potential risks of these novel materials to the environment and human health. In this study, colloidal properties of widely used photocatalytic TiO_2 (P25, Evonik/Degussa GmbH) suspension (TiO_2^{P25}), particularly the sub-100 nm fraction, in commonly used freshwater media for ecotoxicity testings under UV exposure conditions were studied for more than 48 hours by monitoring temporal changes of UV/vis absorbance and with dynamic-light-scattering measurements. The agglomeration and sedimentation kinetics were found strongly dependent on the characteristics of the aqueous media and have important influences on the delivered dosimetry, bioavailability and acute/chronic toxicities of nanoparticle. This study have demonstrated the critical needs of standardized preparation protocols of nanoparticles' dispersion for toxicity testings, which is urgently needed for reliable, reproducible and impartial toxicity tests of manufactured nanomaterials.

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Detection of Single Strand DNA Cleavage by Heavy Metals On FITC Doped Silica BEADs and Its Stability Tests.

고정아, 구진아, 임홍빈

단국대 화학과

Since cause of Itai-itai disease and Minamata disease has revealed , many of research focused on relationship between heavy metals and organ likes brain, kidney, lung and several proteins. But there was not many information about DNA and heavy metal interaction, even though every living things(or organism) have DNA as genetic molecule. Up to now, most of the researches about the DNA-Heavy metal reaction say that heavy metals cleavage DNA by producing ROS. Here, we examined cleavage of single strand DNA by metals in presence of H2O2, and N2 inet state, using FITC doped silica BEADs and Cy5 modified at 5' DNA. For detection, we use Lab built laser induced fluorescence microscope(LIFM) with Photomultiplier tube(PMT) and two kinds of laser (632.8nm He/Ne Laser and 483nm DPSS Laser). And we confirm the FITC doped silica BEADs stability at various pH's and several Hg, Pb, Cd then compare with the intensity of the FITC.

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Analysis of cholesterol in human serum by isotope dilution liquid chromatography-tandem mass spectrometry

신혜선, *이화심

*한국표준과학연구원 바이오임상표준센터 *한국표준과학연구원 바이오/임상센터*

We have developed an isotope dilution liquid chromatography tandem mass spectrometry for the quantitative analysis of cholesterol in serum as a candidate reference method. The advantages of IDMS include a simple sample preparation without derivatization and the use of an isotopic analogue as internal standard. Matrix interferences also can be eliminated by the selective detection of analytes. Isotopic internal standard was cholesterol-3,4-13C2. The LC/MS/MS used in this study was a triple-stage quadrupole mass spectrometer, model API 4000 MS/MS, combined with an Agilent 1200 HPLC through its atmospheric pressure chemical ionization interface. The experiment was operated in positive MRM mode, and cholesterol and cholesterol-3,4-13C2 were monitored at mass transfer m/z 369→147 and 371→149 respectively. The used column was a Thermo ODS Hypersil C18 (100 x 2.1 mm, 3 μm) and column oven temperature was set at 50℃. The mobile phase was 0.05% acetic acid in methanol, and flow rate was 0.3 mL/min. The injection volume was 5 μL. The serum samples were four kinds of KRISS CRMs. In order to verify the measurement method, NIST SRM 909b was analyzed. And the results were agreed well with certified values within uncertainty.

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A Comparison of quantitative analysis for various matrix containing Fe/ Ni by Depth Profiling of Dynamic SIMS.

임원철, *이지혜, **이연희

*KIST 화학분석센터 *고려대 화학과 **KIST 특성분석센터*

Dynamic SIMS has been widely used in an elemental analysis and a depth-profiling for a trace materials existed on the surface because they are highly sensitive to detect a ion current as much as ppm or ppb. However, matrix-dependent secondary ion yields limit the capability of the SIMS technique to obtain quantitative information and there are so many efforts to solve a difficulty to determinate the quantitative analysis due to different matrix effect according to having a different composition. Therefore, we used a Dynamic SIMS and investigated Fe/Ni material to determine the suitable quantitative analysis of thin layer mixed with homogeneous binary alloys such as Fe/Ni, Co/Pt and W/Si. We have obtained a calibration curve to give comparison of quantitative analysis information as much as lower standard deviation. We also have examined for various matrix containing Fe/Ni. The results will be presented and discussed

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Speciation analysis of selenium metabolites in human urine by HPLC-ICP-MS

정지선, 도미송, 박용남

한국교원대 화학교육과

The present study was carried out to separate selenium speciation in human urine sample by HPLC-ICP-MS. Selenium species, trimethylselenonium ion (TMSe), selenocystine (Secys), selenite (SeⅣ), selenourea (SeUr), selenomethionine (SeMet) were seperated on a C8 reversed phase column by mobile phase column of 0.05% nonaflurovaleric acid (ion-pair reagent) and 5% methanol at pH 2.5. The urine sample was only required filtering through a 0.45μm membrane filter and dilution with water in order to measure selenium urinary metabolites.

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Quantitative speciation of selenium by HPLC coupled to post-column isotope dilution analysis ICPMS

도미송, 정지선, 박용남

한국교원대 화학교육과

The purpose of this study is to quantitative speciate of selenium by HPLC inductively coupled plasma mass spectrometer isotope dilution method. The outlet of the chromatographic column was connected through a T-piece where an enriched ^{82}Se spike was continuously added by a peristaltic pump with a flow rate of 0.1 ml min^{-1} and the mixture was nebulized into the plasma.The quantification of selenium was performed by post-column isotope dilution analysis. After reducing the noise level, mathematical corrections were applied to correct for BrH^{+}. Then, the $^{82}Se/^{78}Se$ isotope ratio was calculated and corrected for mass bias. The amount of selenium was calculated by integration of the chromatographic peaks.

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Fabrication of Gold Single Crystal Nanoelectrode

안지희, 김봉수

KAIST 화학과

The small dimensions of the electrode probes increase the temporal and spatial resolutions as well as enhance mass transport rate at the electrodes. We fabricated gold single crystal nanoelectrode. Au nanowires were synthesized by the chemical vapor transport method. The diameters of Au nanowires are 100-200 nm and the lengths of the nanowires are 20-30 μm. Au nanowire was prepared by manipulating and attached to the end of tungsten tip using conducting polymer.

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Determination of trace elements in high purity molybdenum using ICP-MS

정세훈, *박종일

*포항공과대 화학과 *포항산업과학연구원 원천소재 연구센터*

It is very important to know the contents of trace elements in high purity molybdenum. In this study, inductively coupled plasma mass spectrometry (ICP-MS) was used to determination of trace elements in molybdenum. The sample was decomposed by acid digestion methods and then molybdenum was anionized by hydrogen peroxide solution. The trace cation elements in the sample solution were selected by the solid phase extraction using bonded silica gel with benzenesulfonic acid and the elements were determined by ICP-MS. As a result of this anlysical method, many elements such as Ca, Mn, Co, Ni, Cu, Zn, Sr, Cd, Ba, Pb and Bi in molybdenum can be analyzed up to ng/g (ppb) levels.

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Comparison of Diffuse Reflectance Near-infrared spectroscopy and Direct Transmission Raman spectroscopy for the determination of density of polymer.

김재진, 정회일

한양대 화학과

Diffuse reflectance mode can provide the convenience of spectral collection for solid samples when near-infrared spectroscopy is used; however, it has also drawbacks that can negatively influence on accuracy of quantitative analysis. The resulting spectra may represent chemical information related to only sample surface rather than whole same characteristics because the penetration depth of NIR radiation into a sample is not large compared to the size of granular sample. Also, Raman spectra are usually collected by back-scatter mode, which would also provide chemical information related to only surface. The objective of this study is to investigate the possibility of improving the accuracy for density determination of polyethylene (PE) pellet through direct transmission NIR as well as Raman measurement. For NIR measurement, single pellet was located at the center of beam path for spectral collection. For Raman measurement, a laser was illuminated on single pellet and the resulting Raman signal was collected at the opposite side. Both spectral features from NIR and Raman measurements were compared. Finally, the accuracies of density determination from both measurements were compared with the use of partial least squares (PLS) regression.

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Sorption of cobalt by the k-birnessite

강광철, *이석우

*공주대 그린홈에너지기술연구소 *공주대 화학과*

본 연구에서는 K-birnessite 를 환원방법과 졸겔방법으로 합성하였다. EXAFS(Extended X-ray absorption fine structure)를 이용하여 합성된 K-birnessite 에서 Mn 의 산화 상태를 확인하였으며, EDX(Energy dispersive X-ray spectroscopy)를 이용하여 K,Mn,O 의 함량을 측정하였다. 또한 역정적법으로 표면전하를 측정하여 합성된 K-birnessite 의 영전위점을 계산하였다. 계산결과 환원방법으로 합성된 K-birnessite 의 pH_{pzc}=3.5(0.01M)으로 졸겔방법으로 합성된 K-birnessite 의 pH_{pzc}=7.8(0.01M)로 계산되었다. 또한 합성된 K-birnessite 를 이용하여 코발트의 분배계수를 측정하였으며 측정값은 4,800mL/g 값을 나타내었다.

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High Sensitive Nanoarray C-Reactive Protein Array Chip

Md. Shahinul Islam

전북대 화학과

We have demonstrated a method for design a nanoarray protein chip and its application for the high sensitivity detection of C-reactive protein (CRP) in human serum using total internal reflection fluorescence microscopy (TIRFM). The nanoarray of biotin-probe was performed onto 3-mercaptopropyl trimethoxysilane-coated glass coverslip with a spot diameter of ~400 nm within 1 min using a NanoeNabler^{TM}-based surface patterning tool. The unlabeled CRP molecules in human sera were estimated followed by a sandwich fluorescence immunoassay. The linear regression equation y = 0.437x + 84.991 (R = 0.9993) and the limit of detection 50 zM were determined using the standard CRP in the range of 50 zM - 1 fM. The fabricating process of chip was ~2000 times faster than the atomic force microscopy (AFM) based dip-pen nanolithography for the nanoarray. It was 6 X 10^6 times more sensitive than the conventional ELISA.

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*i*PE-MMR: An integrated approach to accurately assign monoisotopic precursor masses to tandem mass spectrometric data

정희정, *김호근, 형석원, 박종문, 문동기, **김경철, 김수진, 이상원

*고려대 화학과 *고려대 고려대 화학과 **고려대 화학*

Accurate assignment of monoisotopic precursor masses to tandem mass spectrometric (MS/MS) data is a fundamental and important step for successful peptide identifications in mass spectrometry based proteomics. Here we describe an integrated approach that combines three previously reported methods of treating MS/MS data for precursor mass refinement. This combined method, “integrated Post-Experiment Monoisotopic Mass Refinement” (*i*PE-MMR), integrates steps: 1) generation of refined MS/MS data by DeconMSn, 2) additional refinement of the resultant MS/MS data by a modified version of PE-MMR, and 3) elimination of systematic errors of precursor masses using DtaRefinery. By combining the synergistic features of each method, iPE MMR increases sensitivity and accuracy in peptide identification when applied to complex high-throughput proteomics data. *i*PE-MMR also allows incorporating additional data processing step(s) or skipping step(s), if necessary, to enable new developments or applications of the tools, as each step of iPE MMR produces output data in a common and conventional format used in proteomics data processing.

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Posttranslational Arginine-Methylation of Lamin A/C during Myoblast Fusion

김수진, 이상원

고려대 화학과

Protein arginine methylation is one of the major posttranslational modifications regulating a various cellular functions such as RNA processing and DNA repair. Recent report showed the involvement of protein arginine methyltransferase (PRMT) 4 in the 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 study focused on the expression and activities of PRMTs during myoblast fusion in primary rat skeletal muscle. Interestingly, ω-NG, NG-asymmetric dimethylarginines (aDMA), and ω-NG, N¢G-symmetric dimethylarginines (sDMA) were found to be consistent during myoblast fusion. However, PRMT1 showed the highest activity during myoblast fusion and maintained thereafter, and PRMT5 reached the highest activity only after myoblast fusion. To identify the proteins modified by such PRMTs 2-DE gel was constructed by the total proteins before and after myoblast fusion, and protein spots on 2-DE with immunoreactive signals against aDMA (Asy 24) and sDMA (Sym 10) were identified by mass analysis. Among the proteins identified, lamin C2 was clarified as a protein to be dimethylated, and we discuss a role of posttranslational arginine methylation for myoblast fusion.

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Label-free Quantitation Using integrated Post-Experiment Monoisotopic MassRefinement (iPE-MMR) and Normalized LC Elution Time (NET) Prediction

김경철, *김호근, 문동기, 정희정, 김수진, 이상원

*고려대 화학과 *고려대 고려대 화학과*

Quantitative analysis of protein expression provides fundamental understanding of the biological changes or biomarker discoveries. In recent years, various stable isotope labeling technique coupled with LC-MS/MS have been widely used for large scale quantitative proteomics. However, several factors, such as the limited number of samples, the complexity of procedures in isotopic labeling experiments, and the high cost of reagents limit the applicability of isotopic labeling techniques to high throughput analysis. Unlike the labeling approaches, the label-free quantitation approach quantifies protein expression across multiple LC-MS/MS analyses directly without using any labeling technique. In this study, we describe label free quantitation approach based on the iPE-MMR we developed and improved, provides highly accurate analyses of massive sets of proteomics data. To increase label free quantitation efficiency, correlation between each LC/MS/MS experiment data should be maximized. Normalized LC elution time prediction technique developed by PNNL was introduced to calibrate elution time of individual LC/MS/MS experiment. Also we make Master Proteome Map which contains all identified peptide's information such as sequence, mass, elution time etc. This master map can be used to give the peptide information to LC/MS/MS features which weren't identified through database search by matching Master Map within certain NET and mass tolerance. In this alignment process, mass and NET refinement is performed using tool developed by PNNL, increasing mass and NET accuracy, enables more accurate alignment between LC/MS /MS experiments.

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Immunoassay by using Z-domain autodisplayed *E.coli* as a solid substrate

박민, *변재철

*연세대 신소재공학과 *연세대 신소재공학부*

The Z-domain of protein A has been known to bind specifically to the Fc region of antibodies (IgG's). In this work, the Z-domain of protein A was expressed on the outer membrane of E.coli by using "Autodisplay" technology as a fusion protein of autotransport domain. The E.coli with autodisplayed Z-domain was applied to the sandwich-type immunoassay as a solid-support of detection-antibodies against a target analyte. For the feasibility demonstration of the E.coli based immunoassay, C-reactive protein (CRP) assay was carried out by using E.coli with autodisplayed Z-domain. The limit of detection (LOD) and binding capacity of the E.coli based immunoassay was estimated to be far more sensitive than the conventional ELISA. Such a far higher sensitivity of E.coli based immunoassay than conventional ELISA was explained by the difference of analyte binding sites and the mobility of E.coli in assay matrix. From the test results of 45 RA patients' serum and 15 healthy samples, a cut-off value was established to have optimal sensitivity and selectivity values for RA. The CRP test result of each individual sample was compared with ELISA which is the reference method for RA diagnosis. From this work, the E.coli with Z-domain was was proved to be feasible for the medical diagnosis based on sandwich-type immunoassay.

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Immunoaffinity layer of SPR biosensor by using outer membrane of Z-domain autodisplayed *E.coli*

박민, *변재철

*연세대 신소재공학과 *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. 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. The LOD of SPR biosensor with the outer membrane of E.coli with Z-domain and intact E.coli outer membrane was estimated to be 1.6 ng/ml, 316 ng/ml, respectively. This result shows 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.

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Capacitive biosensor based on autodisplayed Z-domains for medical diagnosis of meningitis

이주경

연세대 신소재공학과

A capacitive biosensor was developed for the medical diagnosis of menginitis by detection of S100B protein in the patient cerebrospinal fluid (CSF). S100 protein is a calcium-binding protein and consists of two monomers, and it is overproduced during gliosis in patients with Alzheimer disease, Down syndrome and related dementia. Therefore, overproduction of S100B protein was reported to implicate the developmental brain dysfunction. In this work, a capacitive biosensor based on chronoamperometry was applied for the detection of S100B protein. For the improvement of the capacitive biosensor, the outer membrane (OM) layer with autodisplayed Z-domains was used to immobilize anti-S100B protein. In the previous work, we reported that the immunoaffinity layer based on the OM layer could far improve the sensitivity and limit of detection of immunoassays through the orientation control of the immobilized antibodies. For the comparison of sensitivity, different immunoaffinity layers were prepared: self-assembled monolayer (SAM) of 11-mercaptoundecanoic acid combined with covalent coupling of anti-S100B antibodies, physical adsorption of antibodies to the electrode surface. The immunoassay by using the OM layer with Z-domains showed the limit of detection was improved as much as 100-fold higher than the conventional SAM. For the capacitive sensor based on the OM layer with autodisplayed Z-domains, a standard curve at the S100B protein concentration of 1 pg/ml – 10 ng/ml was prepared by using standard samples by spiking S100B protein to CSF. The feasibility of the capacitive biosensor for the medical diagnosis was confirmed by comparison with the test results (n=20) from the conventional immunoassay.

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Protein chip with parylene-H coated surface for improve immobilization efficiency

고혁, 김조일, *변재철

*연세대 신소재공학과 *연세대 신소재공학부*

Parylene H layer was deposited on surface of protein chip to promote its immobilization efficiency. To construct immunoaffinity layer, protein chip made from glass substrate requires surface modifications such as silanization or depositing polymer film on substrates which have been developed1). Through preparing parylene H layer on glass substrate, aldehyde (-CHO) functional groups are exposed on surface of the protein chip. Aldehyde fuctional groups are make covalent bonding with most kinds of proteins and peptides which contain amine groups. Its effectiveness was determined by quantification of immobilized horseradish peroxidase (HRP) compared with polystyrene. For medical diagnostic experiment we detect antibodies against cyclic-citrullinated peptide (CCP) in sera from patients of rheumatoid arthritis (RA) on protein chip by using microarrayer and scanner. The results are compared with those of ELISA assay.

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Parylene-N coating for surface modified SPR biosensor

고혁, 김조일, *변재철

*연세대 신소재공학과 *연세대 신소재공학부*

Surface Plasmon resonance (SPR) biosensor has been applied for the on-line monitoring of a target analyte in complex mixture by using specific interaction between antigens and antibodies. In this work, mainly for reusability of SPR biochip, parlyene thin film was applied as a linker layer on gold surface of the SPR biochip. Parylene is a polymer of p-xylene with good optical properties, chemical resistance from organic solvents and relatively high mechanical strength which are required for the linker layer of SPR biosensor. The SPR effect is known to be the occurrence of an evanescence field by the absorption of incident light at the range of 100nm from the sensor surface and we tested the feasibility of parylene layer of less than 100nm as a linker layer by observation of resonance angle change according to refractive index. Parylene film can be easily coated and removed by oxygen plasma treatment so that SPR biochip can be used repeatedly. The applicability of the parylene film was demonstrated for the detection of anti-CCP(Citrullinated Cyclic Peptide) antibodies in the sera from rheumatoid arthritis(RA) patients.

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Dispersive solid-phase extraction followed by LC-MS/MS spectrometry for the multi-residue analysis of sulfonamides in meat

이경준, 이계호

충남대 화학과

가축의 생산성 및 질의 향상을 증가시키기 위한 목적으로 동물의약품이 과다 사용되어지고 있다. 이는 가축뿐만이 아니라 최종 소비자인 인간에게도 생리학적인 장애 또는 내성이 생기는 문제를 야기 시킬 수 있다. 이러한 문제가 발생하는 것을 예방하기 위해 최대잔류허용량을 규정하고 있으며, 더 효율적이고 정확한 결과를 얻기 위한 방법이 연구되어지고 있다. 이 실험에서는 C18 을 이용한 Dispersive-SPE 방법을 사용하여 경제적이며, 빠른 분석을 할 수 있었다. 또한 매트릭스의 영향을 적게 받고 단시간 내에 분석할 수 있는 HPLC-MS/MS 를 이용하였다. 돼지고기 시료에 sulfonamides 계열의 표준용액을 첨가하여 분석하였으며, 최적화된 전처리 방법과 기기조건을 찾아내었다. 기기의 최적화된 조건을 찾기 위하여 simplex 시스템을 사용하였으며, 회수율 및 검정곡선의 직선성, 재현성에서 만족할 만한 결과를 얻을 수 있었다. 본 실험을 통하여 최적화된 전처리 방법을 개발하여 여러 가지 시료와 분석 물질에 적용함으로써 유해 물질의 분석과 여러 분야에 쉽게 응용될 것이다.

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크로마토그래피를 이용한 모발의 단백질 분석

권종은, 신성재, 이선영, 김정권, 이계호

충남대 화학과

모발의 단백질 중 주 단백질인 케라틴은 절단된 신경의 재생을 촉진하는 것으로 알려져 있다. 이 뿐만 아니라 모발 속에는 다양한 역할을 하는 단백질이 존재하는데, 이를 연구했을 시 의학 및 생물학적 연구와 산업적 응용에 기여할 수 있다. 이 실험에서는 효율적인 모발 분석을 위한 분석방법을 개발하고자 한다. 모발 시료에 chloroform/methanol 을 2:1(v/v)로 첨가시킴으로서 지질 성분을 제거할 수 있었다. 또한 mercaptoethanol 과 tris-HCl, thiourea, urea 를 첨가하여 단백질을 추출시키는 과정을 시행하였다. 이를 HPLC 와 1D-gel 전기영동법 그리고 Maldi TOF-MS 로 분석함으로서 모발 시료 중에 포함 된 케라틴을 분리하고 확인할 수 있었다. 모발에서 케라틴을 분리해 낼 수 있는 최적의 조건을 찾음으로서, 앞으로 모발 분석의 다양한 분야에서 응용될 수 있을 것이다. 향후 이를 기반으로 하여 정상인의 모발과 특정 질병이 있는 사람의 모발을 비교하기 위한 분석 방법을 개발할 계획이다.

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Effects of Elevated Column Temperature of Ultra-high Pressure Microcapillary Liquid Chromatography on Separation Efficiency and Reproducibility

형석원, 문동기, *이후근, 이상원

*고려대 화학과 *가천의과학대 암당뇨연구원*

The increases in separation efficiency and reproducibility of liquid chromatography (LC) are important factors to increase sensitivity of peptide identification and to enhance quantitative analyses of complex high-throughput proteomics experiments, respectively. Here we demonstrate a construction of a column-temperature controlled ultra-high pressure capillary reverse phase liquid chromotgraphy system. This LC system is equipped with a solid phase extraction (SPE) for online backflushing injection/desalting and a long capillary column (360 ㎛ OD, 75 ㎛ ID, 70 ㎝ long), whose temperature is controlled by a semi-flexible heating jacket. Enolase tryptic digests were used as a standard sample to evaluate the separation efficiency. LC retention time reproducibilities at the operation temperatures ranging from room temperature to 60℃ were investigated. With the increased and stable column operation temperature, the LC system exhibited vastly improved reproducibility in LC operation pressures and retention times compared to otherwise non-controlled system. Also with the decreased operation pressure (i.e. back pressure) at an elevated temperature, the system allows using a longer capillary column to improve separation efficiency or using higher LC solvent flows, which improves reproducibility.

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Dispersive solid-phase extraction followed by GC-MS spectrometry for the multi-residue analysis of pesticides in rice

이동욱, 이경준, 권종은, 이계호

충남대 화학과

전 세계적으로 농산물의 생산성 및 질의 향상을 증가시키기 위한 목적으로 농약이 과다 사용되어지고 있다. 하지만 이는 최종 소비자인 인간에게도 생리학적인 장애 또는 내성이 생기는 문제를 야기 시키기 때문에 현재 세계 각국에서 농약에 대한 MRL(Maximum Residue Levels)을 지정하여 규제를 하고 있는 실정이다. 이 실험에서는 ACN 을 이용하여 추출을 하였고, PSA 을 사용한 Dispersive-SPE 방법을 사용하여 경제적이고, 빠르며 많은 시료에 대해 쉽게 전처리를 할 수 있었다. 또한 GC-MS 를 이용하여 다성분 동시분석을 할 수 있는 새로운 분석법을 확립하였다. 시료에 표준용액을 첨가하여 분석하였으며, matrix 에 대한 효과를 최대한 줄이기 위해 matrix matching calibration 을 하였고, 최적화된 전처리 방법과 기기조건을 찾아내었다. 회수율 및 검정곡선의 직선성, 재현성에서 만족할 만한 결과를 얻을 수 있었다. 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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고성능 포토레지스트 제조용 핵심원료인 Adamantane계의 고체 NMR분석 연구

박슬아, 이영일

울산대 화학과

ArF(193nm) 광원을 이용하는 50 나노급 이하에서 사용되는 Photoresist Polymer 용 Monomer 로서 중요한 Adamantane 계 유도체 화합물 합성 중 생성되는 중간물질 및 최종물질을 NMR 실험을 통하여 구조분석을 수행하였다. 기본적인 1 차원(1D) NMR 기법을 비롯하여 공간적 구조의 이해 및 분석을 위해 2 차원(2D) NMR 분석을 수행하여 step 의 안정성 및 정밀성에 대한 정성분석을 수행하였으며, 고상 NMR 분석을 이용하여 시료를 비파괴적으로 분석하였다. 2 차원(2D) NMR 분석의 경우 HSQC 와 COSY 분석법을 사용하였으며, HSQC 분석을 통하여 ^{13}C 와 ^{1}H 핵들의 크로스 피크를 확인하여 각각의 물질의 분자구조와 ^{13}C 와 ^{1}H 의 결합을 밝혀낼 수 있었으며, COSY 분석을 통하여 Adamantane 계 물질의 수소와 수소간의 correlation 에 대한 정보를 얻을 수 있었다.

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Structural analysis of $LiMn_xFe_{1-x}PO_4$ (x = 0, 0.6, 1) with ^7Li magic-angle spinning nuclear magnetic resonance spectroscopy

박슬아, 이영일

울산대 화학과

Solid-state NMR study has been performed to understand relationship between atomic environment and electrochemical performance of $LiMn_xFe_{1-x}PO_4$ (x = 0, 0.6, 1). ^{7}MAS NMR spectra of $LiMn_xFe_{1-x}PO_4$ (x = 0, 0.6, 1) in pristine are characterized by single isotropic peak and broad spinning sideband manifolds, as expected an averaged Li site observing for paramagnetic materials. In case of $LiMn_{0.6}Fe_{0.4}PO_4$, pouch type of cell was constructed to investigate the structural change with the different cut-off voltage regions for study of ^{7}Li MAS NMR. The structural change of $LiMn_{0.6}Fe_{0.4}PO_4$ during the charging process have been observed, which is related with the change of oxidation states from Mn(II) to Mn(III) and from Fe(II) to Fe(III). The isotropic peaks of all samples are accompanied by large and asymmetric spinning sideband manifold, which is arising from bulk magnetic susceptibility broadening and the paramagnetic interaction between the lithium nucleus and transition metal unpaired electrons.

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Preparation of spherical particles based on chiral memory effect

류재정, *Zhang Yi-Jun

*경북대 화학교육과 *Henan Institute of Science and Technology*

Titanium(IV) butoxide, zirconium(IV) oxide chloride, 3-mercaptopropyl trimethyoxysilane, vinyltrimethyoxysilane, octyltrimethyoxysilane 등을 각각 출발물질로 이용하여 졸-겔법 등으로 수 마이크로미터 크기의 구형 titania, zirconia, silica 입자들을 제조하였다. 또한, 앞서 제조한 수 마이크로미터 크기의 구형 titania, zirconia, silica 입자들의 제조 때와 동일한 방법과 출발물질을 써서 각각의 sol 용액에 키랄 메모리 효과를 일으킬 수 있도록 광학적으로 순수한 키랄 물질을 함께 포함시켜 졸-겔법으로 구형입자들을 제조하였다. 제조한 각 입자들을 빈 컬럼에 충전하여 키랄 화합물과 일반 화합물의 HPLC 분리에 적용하였고, 그 차이점을 비교, 고찰하였다.

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Adsorption of Tetracycline in Aqueous solution on Dead pine needles

유구용, 홍성규, *고승원

*삼육대 화학과 *부원중학교*

In this work, the dead pine needles was evaluated for its ability to remove tetracycline from an aqueous solution in a batch process. Equilibrium studies were conducted in the range 7.5-17.5mg/L initial tetracycline concentration, 2-10 solution pH and at temperature of 30°C. The experimental data were analyzed by the Langmuir, Freundlich, Temkin isotherm models. Equilibrium data were fitted to the Freundlich and the Langmuir model. The maximum adsorption capacity of tetracycline on dead pine needles in aqueous solution was 29.586mg/g. The dimensionless separation factor RL revealed the favorable nature of the isotherm of the tetracycline-dead pine needle system

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Fully Stretched DNA Molecules in Nanochannels

김유리, *장락우, 조규봉

*서강대 화학과 *광운대 화학과*

Fully elongated large DNA molecules are well suited for comprehensive whole genome analysis. Among a number of approaches for elongating DNA molecules, nanofluidic molecular confinement has received enormous attentions from physical and biological communities for the last several years. Here we demonstrate a well-optimized condition that a DNA molecule can stretch almost its full contour length: the average stretch is 19.1 μm ± 1.1 μm for YOYO-1 stained DNA (21.8 μm contour length) in 250 nm x 400 nm channel, which is the longest stretch value ever reported in any nanochannels or nanoslits. In addition, based on Odijk's polymer physics theory, we interpret our experimental findings as a function of channel dimensions and ionic strengths. Furthermore, we develop a Monte Carlo simulation approach using a primitive model for the rigorous understandings of DNA confinement effects. Collectively, we present more complete understanding of nanochannel confined DNA stretching via the comparisons to computer simulation results and Odijk's polymer physics theory.

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Artificial neural network study on organ-targeting peptides

정은경, 정동현, *신재민, 최승훈

*(주)인실리코텍 *에스비사이언스(주) 연구소*

We report a new approach to studying organ targeting of peptides on the basis of peptide sequence information. The positive control data sets consist of organ-targeting peptide sequences identified by the peroral phage-display technique for four organs, and the negative control data are prepared from random sequences. The capacity of our models to make appropriate predictions is validated by statistical indicators including sensitivity, specificity, enrichment curve, and the area under the receiver operating characteristic (ROC) curve (the ROC score). VHSE descriptor produces statistically significant training models and the models with simple neural network architectures show slightly greater predictive power than those with complex ones. The training and test set statistics indicate that our models could discriminate between organ-targeting and random sequences. We anticipate that our models will be applicable to the selection of organ-targeting peptides for generating peptide drugs or peptidomimetics.

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Synthesis of novel melanogenesis inhibition agents and *in vitro* assay of its whitening effect

전민, 이다연, 이현상, 천종우, *금내리

*(주)에이씨티 연구소 *단국대 화학과*

Melanin is a polymer of phenol which produces hyperpigmentation in the skin. Melanin synthesis is catalyzed by the enzyme tyrosinase. Ten cyclohexane derivatives were prepared as candidates for new whitening agents. To evaluate the efficacy of the candidates, tyrosinase-inhibitory effect of the candidates on melanogenesis in B16 melanoma cell were investigated and the mRNA expression of TRP-1, TRP-2, and Tyrosinase genes were investigated with using RT-PCR. Western blot was also performed to verify the inhibition of melanogenesis related protein, tyrosinase. The whitening agents suppressed the biosynthesis of melanin and the expression of tyrosinase, TRP-1 and TRP-2 in B16 melanoma cell. However, whitening agents did not inhibitory effect on in vitro tyrosinase activity. These results demonstrated that whitening agents inhibit melanin production which may be dependent on expression in B16 melanoma cell, and it could be apply to the effective skin whitening agents.

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Snap-shot Structure of Caspase-7 Maturation

이영미, *강효진, *정명선, **정상전

*한국생명공학연구원 바이오나노연구단 *과학기술연합대학원대 나노바이오공학 **한국생명공학연구원 바이오나노연구단*

Caspase-7 is one of an apoptotic executioner which cleaves the majority of cellular substrates in apoptotic cells. The enzyme expressed as a proenzyme is activated by other caspases upon cell death signals. Crystal structures of caspase-7 revealed a large conformational difference of caspase-7 active site before and after activation, meaning that the activation induces a large conformational change of loops constituting the active site. In spite of extensive structural and biochemical analyses, a detailed molecular mechanism of the caspase activation remains being solved. We engineered procaspase-7 and crystallized with its specific inhibitor, Ac-DEVD-CHO. Determined structure showed the first procaspase-7 bound to a specific caspase inhibitor, implying that the engineering itself gave caspase-7 a catalytic activity. Surprisingly, two monomers of the dimeric structure showed different conformations representing precursor and matured caspase-7.

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Turn-on Fluorescence Probe based on intrinsic protein fluorescence: A Novel Label-Free Protein Detection by FRET

강효진, *정상전

*과학기술연합대학원대 나노바이오공학 *한국생명공학연구원 바이오나노연구단*

Fluorescence resonance energy transfer (FRET) is a mechanism describing energy transfer between two chromophores. Since its efficiency highly relies on distance between two chromophores. FRET has offered useful tools to quantify molecular dynamics in biophysics and biochemistry, such as protein-protein interactions, protein-DNA interactions, and protein conformational changes. To measure the distance between two molecules by FRET, to date, they must be labeled with fluorescence molecules such as fluorescent proteins, or synthetic fluorescent molecules. But this step is inconvenient and can alter inherent function of target molecules such as proteins, nucleic acids, or synthetic molecules. We have endeavored to develop highly sensitive label-free detection method using FRET based on intrinsic protein fluorescence.

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Molecule-Level Imaging for mRNAs Distribution on a Sectioned Cell

김정숙, 박준원

포항공과대 화학과

RNA localization has emerged as a key process in organizing cellular architecture and function. Detection of the cellular distribution of localized mRNA species is critical in our understanding of the essential cellular process. Atomic force microscopy (AFM) is widely used to observe interaction of biomolecules with piconewton force sensitivity and nanometer positional accuracy. In this study, we obtained the spatial distribution of ammonium transporter AtAMT1;4 mRNA on sectioned pollen at single cell level by 27-acid dendron modified AFM probe. A cone-shaped dendron created appropriate lateral space to hybridize DNA-mRNA pair sufficiently without steric hindrance.

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Metabolite Profiling of ect1 Mutants of Arabidopsis thaliana

강우영

세종대 화학

The ect1 gene of Arabidopsis thaliana has an unknown function in the calcium signaling pathway. The mutant and revertant were constructed and the metabolite profiling was performed to identify those affected by this mutation and whether the revertant successfully restored the cell physiology back to the state of the wildtype. The metabolome would be better than DNA or RNA to describe the cell physiology. Two-dimensional 1H-13C NMR strategy (fast metabolite quantification, FMQ, by NMR) has been applied for identifying and quantifying around 20 most abundant metabolites in the ect1 mutant of Arabidopsis thaliana. Principal component analysis (PCA) showed that the wildtype and revertant were clustered together implying that these two became very similar wile the mutant was farther away from the two. This shows the practical application of 2D NMR based metabolite profiling and PCA.

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Measurement of Affinity between Signal Transducing Proteins through Force Mapping

김일홍, *이미남, **류성호, 박준원

*포항공과대 화학과 *포항공과대 생명과학과 **포항공과대 분자생명과학부*

Atomic force microscopy (AFM) has been used to study specific interaction between signal transducing proteins, Rheb and glyceraldehyde-3-phosphate dehydrogenase (GAPDH). To record the force between them, the proteins were fused with glutathione S-transferase (GST), and immobilized onto the reduced glutathione (GSH) tethered surface. In order to enhance the recognition efficiency and avoid undesirable complication, both AFM tips and substrates were modified with a dendron. To investigate dynamics of these biomolecular interactions, we measured the loading rate dependence of the unbinding forces.

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In Vitro Selection of DNA Aptamers against Nucleocapsid protein of SARS Coronavirus.

조성제, *우혜민, **정용주

*국민대 화학과 효소화학 연구실 *국민대 화학과 **국민대 생명나노화학과*

It is believed that nucleocapsid protein (N) of Severe Acute Respiratory Syndrome (SARS)-CoV is one of the most promising antigen candidates for vaccine design of a newly emerged disease SARS. In this study, DNA aptamers against N protein were isolated from DNA library containing random sequences of 40 nucleotides using a SELEX (systematic evolution of ligand by exponential enrichment) procedure. After 11 rounds of selection, DNA aptamers that bind to the Nucleocapsid protein were isolated and shown to have different binding capacities. Among them, aptamer 3 showed the strongest binding to the N protein and an inhibitory effect on interactions between antigen and antibody, as shown by competitive ELISA. The aptamers that were isolated in this study are expected to be new molecular probes for the investigation of the molecular bases of SARS-Co V diagnosis and treatment.

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The effects of substrate composition on helicase unwinding activity of SARS coronavirus nsP13

이나라, 이아람, *김동은, **정용주

*국민대 화학과 *건국대 생명공학과 **국민대 생명나노화학과*

SARS (Severe Acute Respiratory Syndrome) coronavirus encodes helicase/NTPase, nonstructural protein 13 (nsP13), which efficiently unwinds partial-duplex DNA and RNA. Here, we have investigated the effects of partial-duplex DNA substrates that have different duplex lengths and 5'-overhangs on helicase unwinding activity under single-turnover reaction conditions. The fraction of unwound DNA increased as the length of 5'-overhang increased. On the other hand, the quantity of unwound DNA decreased as the length of the duplex increased. These results indicate that nsP13 requires a long 5'-overhang to unwind longer DNA duplex more efficiently. Additionally, nsP13 recognized gapped DNA and the unwinding activity was enhanced when gapped DNA had a 5'-overhang or the length of gap increased.Acknowledgment: This work was supported by Seoul R&BD Program (10580).

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Molecular Basis of for the Enantioselective Hydrolysis of bβ-Subsituted-γ-acetyloxymethyl-γ-butyrolactones by Burkholderia cepacia Lipase

엄희성, 하현준

한국외국어대 화학과

The favored substrates for hydrolytic reactions mediated by PCL in aqueous media has R configuration of γ-position near the reaction site for γ-((acetyloxy)-methyl)-γ-butyrolactones, trans-β-methyl- and β-ethyl-γ-((acetyloxy)-methyl)-γ-butyrolactones. However, stereochemical preference was reversed for the substrates cis-β-methyl- and β-ethyl-γ-((acetyloxy)-methyl)-γ-butyrolactones, i.e. S configuration of γ-position near the reaction site was favored for the reaction. Furthermore, phenyl substituent at β-position for γ-((acetyloxy)-methyl)-γ-butyrolactone were not accepted as substrate for the reaction. The origin of this reversal stereoselectivity on the PCL mediated enantioselective hydrolysis of β-substituted γ-((acetyloxy)-methyl)-γ-butyrolactones was investigated by molecular modeling. The Umbrella like inversion in γ-position can account for the experimental results.

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OEP7 Recognition of AKR2 as a mediator of protein targeting

이재은, 김일홍, 박준원

포항공과대 화학과

Arabidopsis ankyrin repeat protein (AKR2) as a cytosolic mediator of protein targeting has abilities to recognize the targeting signal of Arabidopsis chloroplast outer envelope membrane protein (OEP7) and to transport OEP7 to the chloroplast. By using AFM, we studied the specific interaction between AKR2 and OEP7 to identify when and how a mediator is recognized. The quantitative measurement of the rupture force between them can show the influence of transmembrane domain/C-terminal positive region (TMD/CPR)-type targeting signals on the networking system of the chloroplast outer membrane.

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Inhibitory Effect of Quercetin with Antioxidant Activity on Matrix metalloproteinase-2 and -9 in HT1080 cells

박인환

동의대 화학과

quercetin is a kind of bioflavonoid contained in several plants. It has been reported to have a variety of medicine effect on allergy, anaphylactic, diarrhea and cancer as well as antioxidant effect. The direct scavenging effect of quercetin on DPPH radical, DNA oxidation, lipid peroxidation and reducing power related to oxidative stress were evaluated in vitro. Furthermore, its antioxidant effect was investigated in human fibrosarcoma cells (HT1080) exposed to hydroxyl radical produced by fenton reaction using TBARS assay. In addition, its inhibitory effect on the activity and expression of matrix metalloproteinase-2 and -9 related to metastasis were determined using gelatin zymography in HT1080 cells. It was observed that quercetin exhibited antioxidant effect on DPPH radical above 4 μM. Especially, quercetin showed an inhibitory effect on lipid peroxidation in vitro, but no effect in live cells. Gelatin zymography assay showed that quercetin inhibited both MMP-2 and MMP-9 activities in the absence of PMA, but only MMP-2 activity in the presence of PMA. While the expression levels of MMP-2 and -9 were reduced by treatment of quercetin at 4 μM, the expression level of tissue inhibitor of MMPs (TIMP-1) was increased in western blot analysis. Quercetin attenuated PMA-induced activation of p-p38, a mitogen-activated protein kinase. In conclusion, these findings suggest that quercetin can be applicable to chemoprevention for metastasis.

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Rational design for improving amidase activity of *Candida antarctica* lipase B

김주현, 박성순

성신여대 화학과

Lipases have been used in many applications, such as preparation of chiral alcohols and esters, because they are highly selective and reactive. However, most lipases cannot hydrolyze amides although their active sites are similar to those of serine-protease that catalyze hydrolysis of amides. Recently, we proposed molecular basis for the enhanced lipase-catalyzed *N*-acylation of 1-phenylethanamine with methoxyacetate. We hypothesized that the hydrogen atom connected to the nitrogen atom of the amine substrate may interrupt formation of the key hydrogen bond between the catalytic histidine and the nitrogen atom of the substrate. This disruption could be avoided by using methoxyacetate as an acyl donor. The methoxy group of the acyl donor can hydrogen bond to the nitrogen atom and thus the proton does not interrupt the key hydrogen bond. In this study, we introduced a residue to serve a similar role to the methoxy group into a lipase. We prepared several mutants of *Candida antarctica* lipase B (CAL-B) to construct a hydrogen bond between the residue introduced and the nitrogen atom. One of the mutant enzymes showed a nine-fold enhanced specific activity toward hydrolysis of *p*-nitroacetanilide compared to the wild-type enzyme.

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Purification of bioactive peptide with contractile activity on the smooth muscle from squid gill (*Todarodes pacificus*)

조은희, 고혜진, 김혜림, 우경은, 박남규

부경대 생물공학과

A bioactive peptide with contractile activity was isolated from the gill of squid, *Todarodes pacificus*, using the smooth muscle of the squid as the bioassay system. The acified extract of squid' gill was forced through the Sep-pak C_{18} cartridge using stepwise gradient with increasing the percent of methanol (10%, 60%, 100%) containing 0.1% TFA.Among of them the 60% methanol fraction showed the highest contractile activity on the smooth muscle from squid at each extracts. Then 60% methanol fraction was purified by gel chromatography, ion-exchange and C_{18} reversed phase HPLC.Finally, a peptide was obtained in isocratic condition 19 % CH_3CN at a flow rate of 0.5 ml/min. This peptide was analyzed by ESI Q-TOF MS/MS and amino acid sequencing. The molecular weight of this peptide was 1600 Da and composed of 14 amino acid residues.

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Purification and characterization of a novel neuropeptide with contractile activity on the smooth muscle from squid brain (*Todarodes pacificus*)

조은희, 고혜진, 김혜림, 우경은, 서정길, 박남규

부경대 생물공학과

A novel neuropeptide with contractile activity was isolated from the brain of squid, Todarodes pacificus using the digestive gland of the squid as the bioassay system. To purifiy neuropeptide the acified extract was partially purified with Sep-Pak C_{18} solid phase extraction cartridges using stepwise gradient with increasing the percent of methanol (10%, 60% and 100%) containing 0.1% TFA. Contractile activity was recovered in the 60% methanol fraction and this fraction was further purified by ion-exchange and C_{18} reversed-phase HPLC.Finally a new peptide was obtained in isocratic condition of 21% CH_3CN at a flow rate of 0.5ml/min. This peptide was analyzed by ESI-Q TOF MS/MS and Edman degradation amino acid sequencing. The molecular weight of this peptide was 1559.9Da and is composed of 14 amino acid residues. A neuropeptide was isolated from brain of squid(SB) was synthesized by the solid phase method. To compare the homology between native and synthetic peptide.From these result, the C-terminal portion of SB turned out to be $-NH_2$. SB showed threshold response at 10^{-9} M and the $E_{max}$was 167.93% at $5X10^{-7}$ M.In order to investigate the structure-activity relationship, various analogus of SB were synthesized by solid phase method. They are analogs with is deleted one by one amino acid residue in N- and C-terminus. Contractile activities of all peptides were measured by using the smooth muscle of squid. N-terminal delete analog(1-DES SB) showed a similar contractile effect compared with that of SB-NH_2, while, other analogs was inactive. These result indicate that 1-DES SB is the minimum structure required for the contractile activity on the smooth muscle of squid.

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Screening for Drug-Resistant Mutation of HBV

정덕현, 안영창, 조민호, 윤일규, 이은영, 김진호, *장원철

*단국대 화학과 *단국대 첨단과학대학*

Lamivudine is a major drug approve for treatment of HBV infection and a specific inhibitor of the viral polymerase and reverse transcriptase. But, in long-term lamivudine therapy, about 6 month ~ 1 year after, over 14% drug-resistant mutations were found in treated patients. In clinic system, drug-resistant test or screening is very important for therapy. In this study, we propose a useful tool for drug-resistance HBV screening by denaturing high performance liquid chromatography(DHPLC). It have been detected successfully for substitution, insertion, deletion of HBV DNA. As a results, we could identify wild type HBV DNA and the other types such as rtL180M by DHPLC. Application of this high throughput assay(DHPLC) into clinical use should enable earlier diagnosis and better treatment of lamivudine resistant HBV. Further study, we need to test more patient samples screening for other resistant mutations in HBV reverse-transcriptase gene.

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Polymorphism Screening of the DNA Repair Gene XRCC1 in Lung Cancer

이은영, 안영창, 조민호, 윤일규, 정덕현, 김진호, *장원철

*단국대 화학과 *단국대 첨단과학대학*

Recent evidence that some DNA-repair functions are haploinsufficient adds weight to the notion that variants in DNA-repair genes constitute part of the spectrum of defects contributing to cancer risk. DNA repair plays a critical role in protecting the genome of the cell from insults of cancer-causing agents, such as those found in tabacco smoke. Defects in the repair and maintenance of DNA increase risk for cancer. X-ray cross-complementing group 1 protein (XRCC1) is involved with the repair of DNA single-strand breaks. We investigated the relationship between the codon 399 polymorphism in XRCC1 gene and lung cancer. In this study, polymorphism screening of XRCC1 was performed for 109 lung cancer parients of breast disease by denaturing high performance liquid chromatography (DHPLC). DHPLC is a sensitive and fast method for the detection of mutations which has been successfully used for mutation screening in several disease-related genes. Through this study, we identified that Korean lung cancer has polymorphism type of Arg399Gln amino acid changes in the XRCC1 gene. Further study, we will identify that association between the codon 399 polymorphism in XRCC1 gene and EGFR mutation in lung cancer.

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Rapid and sensitive detection of genetically modified soybeans.

김진호, 안영창, 조민호, 윤일규, 정덕현, 이은영, *장원철

*단국대 화학과 *단국대 첨단과학대학*

The most generally accepted GMOs detection methods are based on the polymerase chain reaction (PCR), because of the high stability of the DNA molecule and the capability to amplify specific DNA fragments from highly processed materials. But, loop mediated isothermal amplification (LAMP), that amplifies DNA with more high specificity, efficiency and rapidity under isothermal condition. In this study, when compared PCR and LAMP from same conditions, undiluted DNA (30ng/ul), 10^{-1} ~ 10^{-10} (ng/ul) of GM soybeans DNA were amplified, as a result, LAMP method is expected to detection of GM soybeans with high selectivity, specificity, efficiency and rapidity.

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Thermal stability of liposomes related to mechanical stiffness, phase behavior, and its curvature

이여라, 은채정, 하영은, 서영수

세종대 나노공학과

We investigate thermal stability of liposome in terms of lipid mole fraction and also non-lipid ingredients such as cholesterol and surfactants, where lipids and ingredients are selected on the basis of their charge density, morphology, and hydrophobicity. SUV were prepared by a multiple extrusion method through a membrane with 50nm pore size. Basic parameters extracted from the studies of Langmuir monolayer at the air/water interface and supported bilayer and multilayer are applied for interpretating the stability of liposome. Experimental tools used in this study are Langmuir trough for surface pressure-area isotherms, Dynamic Light Scattering for hydrodynamic radius and its distribution of SUV, and X-ray reflectivity and grazing incidence angle X-ray diffraction for phase behaviors of supported bilayer and multilayer. In addition we will discuss the effects of curvature of liposome on its thermal stability.

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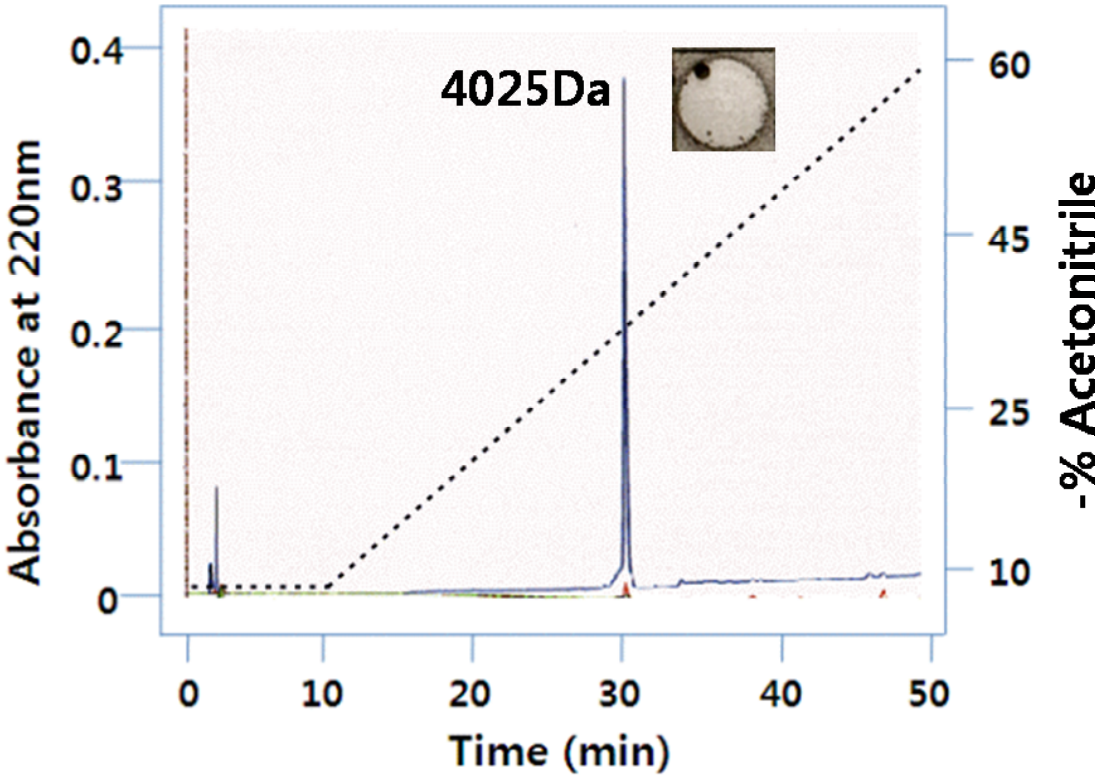
PURIFICATION AND CHARACTERIZATION OF A NOVEL ANTIMICROBIAL PEPTIDE FROM THE MUSCLE OF STARFISH (*Asterina pectinifera*)

우경은, 고혜진, 김혜림, 조은희, 서정길, 박남규

부경대 생물공학과

The acidified muscle extract of starfish showed strong antimicrobial activity against *B. subtillus* and *E. coli* D31. To purify antimicrobial peptide, the acidified extract was partially purified with Sep-pak C18 solid-phase extraction cartridges using stepwise gradient with increasing the percent of acetonitrile (10%, 60%, 100%) containing 0.1% TFA. Antimicrobial activity was recovered in the 60% acetonitrile fraction and this fraction was further separated by sequential reversed-phase high performance liquid chromatography (C4, C18, Phenyl column). Antimicrobial material was purified to homogeneity and its activity was completely lost after treatment with the trypsin. This result suggests that the purified material is a peptide. For the characterization of the purified material, the moleculur weight and amino acid sequence analysis were performed by MALDI-TOF MS and Edman degradation. The moleculur weight of this material turned out to be 4025 Da and the amino acid sequence analysis is in processing. Fig. Final purification of the antimicrobial material by HPLC using Phenyl column. The peak was eluted with the gradient of water and acetonitrile containing 0.1% TFA : 10 -> 50 % acetonitile over 50 min, 1 ml/min, 220 nm. The moleculur weight of the purified material was 4025 Da and the antimicobial assay was tested against *B. subtillus* KCTC1021.



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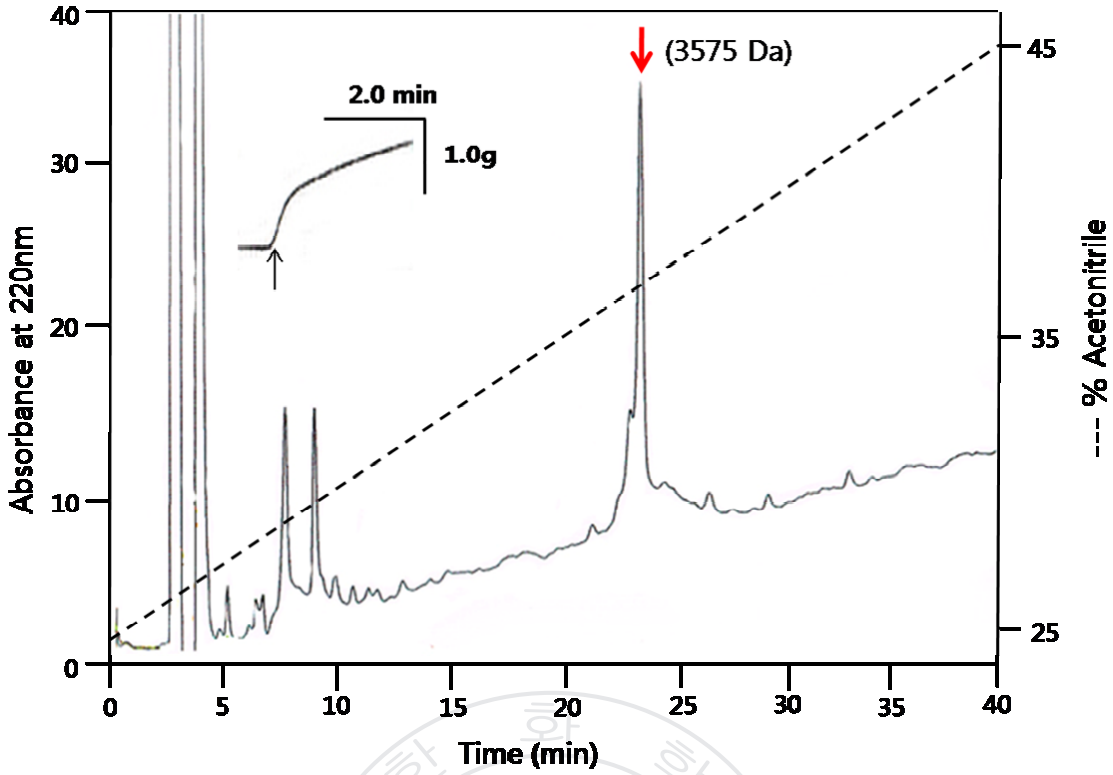
발표종류: 포스터, 발표일시: 목 15:00~17:00

PURIFICATION AND CHARACTERIZATION OF A NOVEL NEUROPEPTIDE FROM THE TUBEFEET OF STARFISH, *Asterina pectinifera*

김혜림, 고혜진, 우경은, 조은희, 서정길, 박남규

부경대 생물공학과

A novel neuropeptide with contractile activity on the dorsal retractor muscle (DRM) of starfish was isolated from the acidified tubefeet extract of starfish, Asterina pectinifera. To purify contractile peptide, the acidified extract was partially purified with Sep-pak C18 solid-phase extraction cartridges using stepwise gradient with increasing the percent of acetonitrile (10%, 60%, 100%) containing 0.1% TFA. The contractile activity was recovered in the 60 % acetonitrile fraction. This fraction was further separated by C4 reversed phase, gel-filtration and C18 reversed phase HPLC and a contractile active peptide was purified to homogeneity. For the characterization of the purified peptide, the moleculur weight and amino acid sequence analysis were performed by MALDI-TOF MS and Edman degradation. The moleculur weight of this peptide turned out to be 3575 Da and the amino acid sequence analysis is in processing. Fig. Final purification of the contractile peptide by HPLC using CAPCELL PAK C18 column. The peak was eluted with the gradient of water and acetonitrile containing 0.1% TFA : 25 -> 45 % over 40min, 1.0 ml/min, 220 nm and the contractile activity was tested on the dorsal retractor muscle (DRM) Purified peptides were applied at time indicated by down arrow.



대한화학회 THE KOREAN CHEMICAL SOCIETY

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Characterization and structure-activity relationship of SF-CT with relaxing activity on the DRM from the starfish, Asterina pectinifera

고혜진, 조은희, 김혜림, 우경은, 박남규

부경대 생물공학과

In previous study, We were SF-CT was isolated from the starfish by using the dorsal retractor muscle (DRM) of starfish (*Asterina pectinifera*) as the bioassay system. The sequence of the purified peptide was analyzed by an automated amino acid sequencing and MALDI-TOF mass spectrophotometry. Molecular ion peak in the MALDI-TOF mass spectrum of the peptide was displayed 3655 Da. The primary structure of the purified peptide was determinated as SGTGXTQFSG XAQLKVGQDALSRVLADSNSRFGSGGP-NH_2. To investigate the complete primary struc ture of SF-CT, SF-CT were synthesized, and chemical and pharmacological properties of the synth etic peptides were compared with those of native peptides. Both native peptide and the synthetic peptide indicated identical behaviors on the reverse-phase HPLC chromatogram, in which the primary structure of native peptide turned out to be SF-CT. Synthetic SF-CT showed relaxing activity at a thr eshold concentration of approximately 10^{-12} M and the Emax was 87.7± 2.5 % at 10^{-5} M on the starfish DRM. In order to investigate the peptide structure-activi ty relationship, various analogs of SF-CT were synthesized by solid phase method. The analogs are deleted one by one the amino acid residues in N-terminus and substituted by Ala in Cys5 and Cys11 of SF-CT ([A5,11]-SF-CT) and deleted Ala^{20} residue (20A-DES-SF-CT). Relaxing activities of all peptides were measured by using the starfish DRM. N-terminal deleted analogs showed a similar rel axing effect compared with that of SF-CT, while, [A5,11]-SF-CT, 20A-DES-SF-CT was inactive eve n at higher concentration, 10^{-5}M. The results when comparing N-terminus analogs with DRM showed that Cys-Cys bond played an important role in receptor-affinity.

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Fabrication and release of BSA-FITC incorporated calcium phosphate microspheres

고일환, *장정호

*인하대 화학공학과 *한국세라믹기술원 바이오IT융합센터*

This work will present the fabrication of BSA-FITC incorporated calcium phosphate at room temperature for applying to bone material. The key process for the fabrication of CaP microsphere is based on water-in-oil emulsification and the use of urease to adjust the reaction pH upto neutral through the decomposition of urea.Obtained BSA-FITC incorporated calcium phosphate microspheres are shown the homogeneous particles sizes in the range of 200-300 ㎛. We conformed decomposition of urea by urease for FT-IR and incorporated BSA-FITC for confocal fluorescene microscopy. We perfomed release of BSA-FITC incorporated in CaP microsphere by measuring amount of BSA-FITC in supernatants depending on storagetime at 280nm and 562nm(micro BCA Protein Assay). We believe that these materials are potentially appllied to the biomedical fields as an injectable bone filler with the controlled drug release materials.

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Ortho ,para Disubstituted benzylidine 2,4 thiazolidinedione as a PTP 1b inhibitor and PAAR activator.

Kafle Bhooshan

인하대 화학과

Compound 18I shows the dual nature as a PTP 1b inhibitor in submicromolar range and PPAR activator as a stablished activator like troglitazone, rosiglitazone and pioglitazone. In vivo, it acts as an antiobesity and hyperglycemic agent

한국화학회 THE KOREAN CHEMICAL SOCIETY

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DNA chip Analysis using Atomic Force Microscope

권성홍, 이윤희, *고현경, *김동욱, 박준원

*포항공과대 화학과 *가톨릭대 분자유전학연구소*

DNA chip is very useful tool for detecting cDNA or cRNA. Since the DNA chip contains tens of thousands of probe DNA microarrays which can hybridize each specific target gene, it can detect a large number of genes at once. Currently researchers are applying DNA chip to many types of investigation, such as gene expression profiling, mutation analysis, and gene sequencing. In the development of the analytical methods based on DNA hybridization, however, there are still technical limitations, like DNA labeling process and DNA amplification. Probe-target hybridization is usually detected and quantified by fluorophore labeled target DNA, but sometimes photobleaching and background signal can make uncertainties of DNA quantification. Moreover, target DNA amplification cannot be avoided due to reaching the detection limit of DNA chip. Here we offer a new approach to DNA analysis on DNA chip surface using atomic force microscope (AFM) that can detect small amount of target DNA without any target labeling and amplification. On the dendron surface which can give sufficient space to hybridize, the target cDNA is detected by measuring hybridization force with probe DNA. This approach will help to alleviate the limitations of common DNA detection technologies, and bring new insight into the studies about cancer diagnosis and gene expression profiling.

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Pyrosequencing using a pyrophosphate sensor

권혁성, *김다래, **홍종인, ***안대로

*KIST 의과학센터 *고려대 생명공학과 **서울대 화학부 ***KIST 생체과학부*

Pyrosequencing is a DNA sequencing method based on quantitation of pyrophosphate produced during DNA polymerization; the amount of pyrophosphate produced is proportional to the intensity of bioluminescence obtained in a reaction cascade with four enzymes trigered by the pyrophosphate. In this presentation, we tested a chemical sensor of pyrophosphate for possible replacement for the expensive enzyme-based reporting system in pyrosequencing.

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Production and NMR Structural Studies of Bovine Lactophoricin

박태준, 김지선, 김용애

한국외국어대 화학과

Lactophoricin (LPcin-I) is a 23-amino acid peptide that corresponds to the carboxyterminal 113 to 135 region of component-3 of proteose peptone (PP3), a minor phosphoglycoprotein found in bovine milk. It has been reported that LPcin-I has antibacterial activity and a cationic amphipathic helical structure, but its shorter analogous peptide (LPcin-II), a 17-amino acid peptide, corresponding to the 119 to 135 region of PP3 does not display antibacterial activity. In fact, it was interestingly known that LPcin-I and LPcin-II have similar charge ratios and identical hydrophobic/hydrophilic sectors, according to their helical wheel projection patterns, and both peptides show cationic amphipathic helical folding and interact with membranes. However, it is known that only LPcin-I incorporates into planar lipidic bilayers by forming voltage-dependent channels. In this study, we cloned and expressed two recombinant peptides in the form of inclusion bodies to understand the structure-activity relationship of these peptides. Fusion proteins were purified by Ni-NTA affinity chromatography under denaturing conditions, and recombinant LPcin-I and LPcin-II were released from fusion by chemical cleavage. Final purifications were achieved by preparative reversed-phase HPLC. Using these methods, we obtained several tens of milligrams of uniformly and selectively 15N labeled peptides per liter of growth, which was sufficient for solid-state NMR spectroscopy. The peptides were identified by polyacrylamide gel electrophoresis and mass spectroscopy. Further integrity and structural information was obtained by circular dichroism, solution and solid-state NMR spectroscopy in the membrane-like environments.

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High-yield Expression and Purification of Transmembrane region of Ion Channel-forming Amyloid-beta Protein Solid-state NMR Structural Studies

박태준, 임수연, 김용애

한국외국어대 화학과

Up to now, enormous progress has been made towards understanding of the cell biology and plaque properties of Alzheimer's disease. But globular and nonfibrillar Amyloid-beta proteins are uninterruptedly produced during normal cellular metabolism and are also present in Alzheimer tissues. In addition to it, small nonfibrillar Amyloid-beta protein alone is sufficient to cause cellular degradation. One of the possible mechanisms for Amyloid-beta protein toxicity suggests that nonfibrillar Amyloid-beta protein form calcium-permeable ion channels in the cell plasma membrane. These channels might allow excessive calcium influx and disrupt the normal cellular calcium homeostasis. But little is known about the transmembrane region and the channel structure of Amyloid-beta protein as an ion-channel protein except a theoretical model.This is due to challenges in the expression, purification, and sample preparation of eukaryotic membrane proteins. To determine the threedimensional structures of the intact transmembrane domain from human APP (hAPP-TM) and to elucidate the structure and formation mechanisms of the hAPP channel, the isotopically labeled protein must be produced and purified in sufficient quantity. Here, we describe a procedure whereby the hAPP-TM peptide, comprising residues 692–723 of hAPP, was successfully expressed and purified sufficiently to perform NMR analysis. To increase expression levels of the target protein, we designed a construct containing two tandem repeats of the target gene. The fusion protein was expressed in the form of inclusion bodies, and purified on immobilized nickel affinity chromatography. Final purification of hAPP-TM was achieved by preparative reversed-phase high performance liquid chromatography (HPLC). The final yields of purified hAPP-TM were around 5 mg/lL of M9 minimal media. Proper folding of the hAPP-TM in a micellar environment was optimized and measured by heteronuclear NMR spectra recorded on a uniformly 15N-labeled sample.

Structural information of the hAPP-TM in the membrane-like environments was obtained by circular dichroism (CD), solution and solid-state NMR spectroscopy.

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Studies of methyl coenzyme M reductase system

김연주, 원호식

한양대 응용화학과

Ni(II)-containing coenzyme F430 catalyzes the final step of methanogenic process and produce the methane and a heterodisufide(CoM-S-S-HTP). Methyl CoM reductase system consists of $\alpha_2\beta_2\gamma_2$dimer (MW=300,000 dalton) with two catalytic active sites. F430, Methylated Coenzyme M, a reducing agent HS-HTP are major novel enzymes involved in methane production via activated square pyramidal organic-nickel complex. Three catalytic processes are set as follow: resting step, complex formation step, and methane production step. These catalytic processes associated with the conformational changes and oxidoreduction state of Ni(II)-containing corphinoid were monitored by detail molecular dynamic computations. Methods in computations, conformational changes and NMR observations for F430 are discussed to assess the mechanistic pathway in detail.

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Studies of Mycobacterium tuberculosis adenylate kinase and it's double mutant (A11S/E112K), by NMR and molecular dynamics

한승원, 우선희, 최현주, 우민희, 원호식

한양대 응용화학과

Adenylate kinase from Mycobacterium tuberculosis (AKmt), a protein of 181 residues is short variant with low similarity with the eukaryote cytosolic AKs. It is an essential enzyme for bacterial survival and it's catalytic activity is lower than other AKs((AKe, AK1 etc). But recently we found that catalytic activity of two point double mutant(A11S, E122K) of AKmt, AKmtDM was 12 fold increased. In this work, a solution-state NMR approach and Molecular Dynamics simulation were used to probe the structural and dynamic distinction of AKmt and AKmtDM. Firstly, chemical shift analysis of AKmtDM, using the ^{1}H-^{15}N HSQC experiment, show that ATP binding P-loop(7-13), LID domain and surrounding residues of LID domain (115~135) are slightly perturbed($\delta w \approx 0.1$~03ppm). It suggests that AKmtDM backbone structure is differ from AKmt at ATP binding active site and it's structural perturbation maybe induce significant backbone rearrangement and eventually produce the difference of catalytic activity. To closely understand structural and dynamic motion, we perform 10ns MD computer simulation using the explicit water system. Principal component analysis of MD simulation performed on AKmt and AKmtDM shows that the sum of the eigenvalues related to the overall fluctuations is 4.85nm^2 for AKmtDM and 1.3 fold larger than that of AKmt. Moreover, simulation in AKmtDM reveals that the first 3 mode account for 70% of the total fluctuation. The main contribution to the overall enzyme fluctuation is given by the LID, AMP-binding domain and P-loop (AKmt is mainly AMP-binding domain motion) and especially fluctuations of LID and P-loop in AKmtDM contribute critical conformational transition. MD simulation also show that stable salt bridge K122-E118 at the LID domain interface and hydrogen bonding R123-S11 LID-Core interaction stabilize the open conformation. These results provide specific knowledge about structural dynamic motion of AKmt/AKmtDM and more generally suggest that molecular dynamics simulation can provide valuable information for identifying catalytic activity

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Conformational studies of the mimotope peptide of apolipoprotein B4i by NMR spectroscopy

Khan asghar, 원호식

한양대 응용화학과

Apolipoproteins are protein components of lipoproteins exhibiting major roles in the transport of plasma lipids and used clinically for the of coronary artery disease. A number of mimetic peptides of apolipoproteins were screened from the phage-displayed random peptide library by using a biopanning method. The mimetic peptides were recognized by the monoclonal antibody against apo B-100 specific monoclonal antibody was $(CRNVPPIFNDVYWIAF)_4$ (B4i). Theses amino acid sequences of peptides are notin original antigens apo B-100. Compared with primary arrangement of amino acid using of BLAST search, B4i were confirmed 40% homology with apo B-100. In this study, ^{1}H-NMR and 2D NMR(COSY, TOCSY, NOESY) experiments were accomplished andsignal assignments of mimotope peptides were made. Distance of numerous proton paris were obtainedbased on the NOE cross peak intensities of NOESY spectrum. On the basis of these distance data, distance geometry(DG) and molecular dynamic(MD) were carried out to determine the tertiary structure of mimotope B4i. DG structures of three mimotope B4i were low penalty value 0.3 ~ 0.6 $Å^2$, and the total RMSD obtained upon superposition of all atoms were in the range 0.5 ~ 1.5Å. Mimotope B4i has a similar 3_{10}-helix structure from Ile^7 to Trp^{13}.

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Thermostable Aspartate Aminotransferase from Hyperthermophilic archaeon, Aeropyum pernix K1

이대경

중앙대 화학과 생명분자화학연구실

Aspartate aminotransferase (AAT, EC.2.6.1.1), the well known pyridoxal 5`-phosphate dependent enzyme, catalyzes the reaction of L-aspartate and α-ketoglutarate to glutarmate and oxaloacetate. This catalytic reaction is essential for nitrogen and carboxylic cellular metabolism. Aeropyrum pernix K1 is an aerobic, hyperthermophilic archaeon that grows optimally at 90~95℃. This archaeon are expected to produce the thermostable enzymes, and the enzymes are not only thermostable but also resistant to a variety of organic solvents. The gene of APE2423, the coding sequence of aspartate aminotransferase from Aeropyrum pernix K1 was cloned using specific primers by PCR. The PCR product was inserted into pGEX-KG, the expression vector and expressed in BL21 codon plus, the host cell. The crude extracts of the cells were subjected to affinity chromatography with GSH-Sepharose. The recombinant fusion protein of AAT-GST was treated in thrombin, and it was purified by affinity chromatography. The purified ApAAT had molecular mass of 42kDa on SDS-PAGE. The enzyme activity was confirmed to measure the RED-OX change of NADH that is resulted from coupling reaction between oxaloacetate and malate dehydrogenase at 340 nm. The optimum pH and temperature of the recombinant aspartate aminotransferase on Asp-α-ketoglutarate conjugation reaction by the enzyme were pH 8.0 and 85℃, respectively. The recombinant aspartate aminotransferase was highly stable against high temperature. Further studies are underway to elucidate the detailed physiological functions of Aeropyrum pernix K1 aspartate aminotransferase and to utilize this enzyme in medicine and bio-industrial processes

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Detection of human pandemic influenza A (H1N1) viruses

김태선, thuan-nguyenvan

한림대 화학과

A novel strain of influenza A (H1N1) was identified in April 2009 and developed into a pandemic flu by June 2009. Pandemic Flu rapidly spreaded around the world so easy and rapid detection of H1N1 out of seasonal Flu was awaited to carry out appropriate patient and public health management. Thus, we developed flu detecting DNAchip with new probes which can hybridize RT-PCR products of H1N1 and seasonal flu at room temperature in less than 1 hr.

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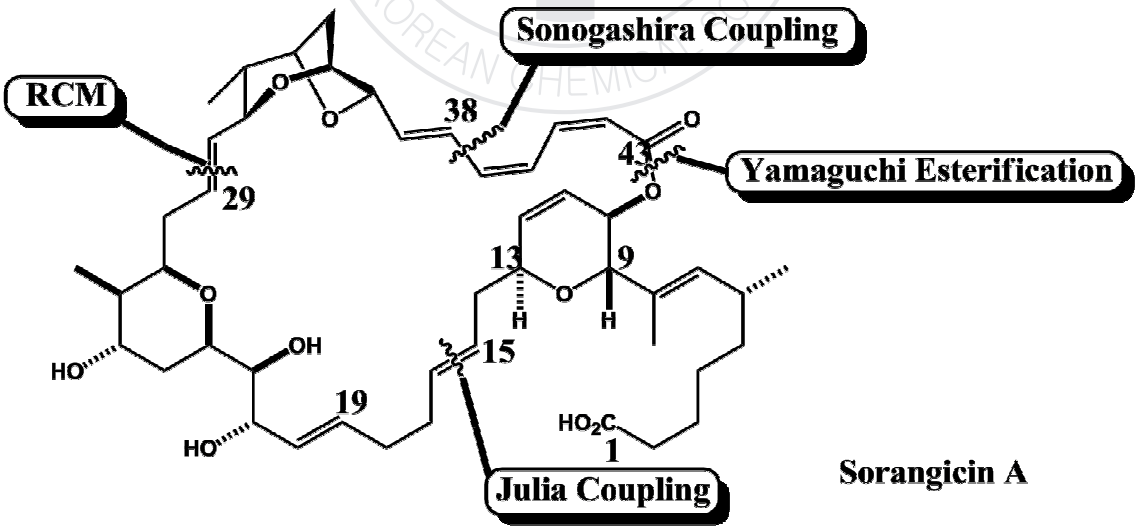
Synthetic Study of (+)-Sorangicin A : Construction of the C1-C15, C16-C29, and C30-C37 Fragments

이성로, 이효원

충북대 화학과

Sorangicin A is a new type of macrolide polyether antibiotic isolated from the gliding bacterium Sorangium cellulosum. The Fragment of C1-C15 was constructed using RCM reaction. The Fragment of C16-C29 was synthesized using asymmetric alkylation and allylic etherification with a Rhodium catalyst. The C30-C37 fragment was prepared utilizing the Sharpless asymmetric epoxidation and the ring opening of epoxide under acidic condition. The details of our synthetic work will be presented



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Synthesis and characterization of a novel fullerene derivative for organic solar cells

미동보, 황도훈, *윤성철, **신원석, ***이창진, ****문상진

*금오공과대 응용화학과 *한국화학연구원 화학소재연구단 **한국화학연구원 에너지소재연구센터 ***한국화학연구원 화학소재연구부 소재7팀 ****한국화학연구원 신화학연구단*

A novel fullerene derivative has been synthesized and characterized. The new derivative has good solubility in common organic solvent such as toluene, chlorobenzene and 1, 2-dichlorobenzene. Photovoltaic devices have been made using the new fullerene derivative as electron acceptor in the fabrication as bellow: ITO/ PEDOT: PSS/ Active layer / LiF / Al. The ratio of the electron donor (P_3HT) and acceptor were 1:0.5, 1:0.7 and 1:1. The enhancement of Voc has been found since the LUMO level of the new derivative increased. High power conversion efficiency (PCE) has been found after annealing at 150°C for 5min with 80nm thickness for the active layer.

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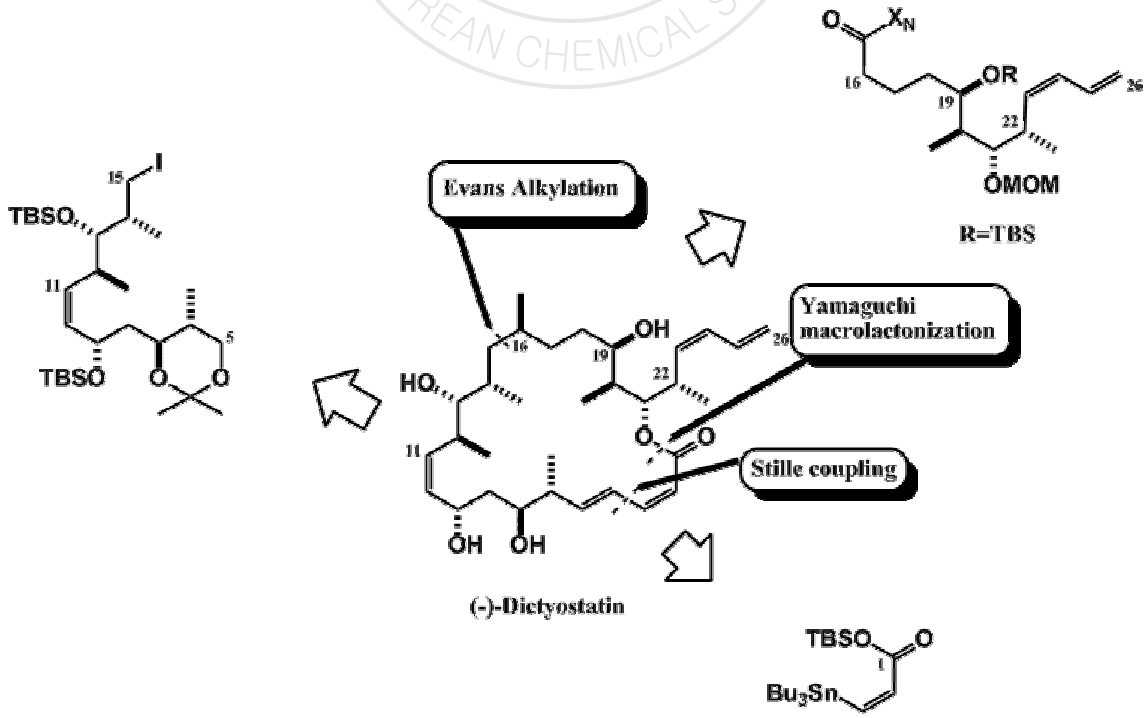
Synthetic studies of C5-C15 and C16-C26 subunits of (-)-dictyostatin and their coupling

우대구, 이효원

충북대 화학과

The 22-membered antimiotic macrolide (-)-dictyostatin was first isolated from the marine sponge Spongia sp. by Pettit and co-workers in 1994 and is structurally related to discodermolide. Dictyostatin inhibits the growth of human cancer cells by stabilizing tubulins like taxol. We achieved the asymmetric synthesis of C16-C26 northern part and C5-C15 western part of (-)-dictyostatin using chemical manipulations such as the ring-closing metathesis (RCM) upon silicon tethers, the Sharpless asymmetric epoxidation, the Cope elimination, and the Evans aldol reaction. Synthetic details will be disclosed.



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발표코드: **Ⅰ37P192포**
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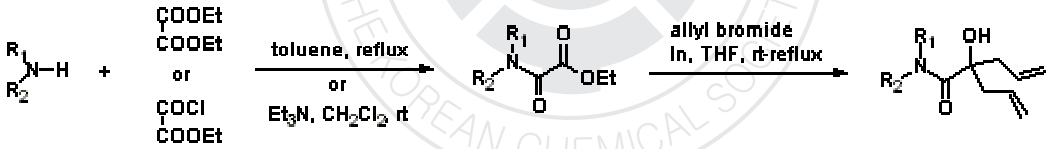
발표종류: 포스터, 발표일시: 목 10:30~12:30

Synthesis of diallyl carbinols via the In-mediated allylation of oxalic amide-esters

김유미, 김성환, 김재녕

전남대 화학과

An efficient synthesis of diallyl carbinols was carried out by the reaction of allylindium reagents and esters activated with various amides. Although simple esters are not reactive toward allylindium reagents, esters activated with another carbonyl group of amide reacted readily and produced synthetically useful diallyl carbinols.



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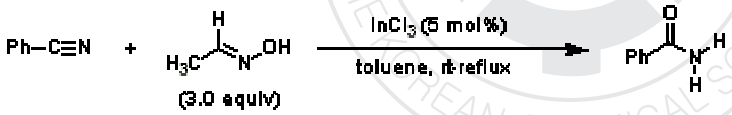
An efficient $InCl_3$-catalyzed hydration of nitriles to amides: Acetaldoxime as an effective water surrogate

김은선, 박보람, 김재녕

전남대 화학과

An efficient $InCl_3$-catalyzed hydration protocol of nitriles to amides was developed. The reaction was carried out in toluene at refluxing temperature with the aid of acetaldoxime as an effective water surrogate to produce amides in high yields. In addition, a one-pot conversion method of aldoxime to amide was developed by using a similar concept.



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발표종류: 포스터, 발표일시: 목 10:30~12:30

Facile synthesis of *N*-tosyl *aza*-Baylis-Hillman adducts of acrylamide *via* a Pd-catalyzed hydration of nitrile to amide

김은선, 이현승, 김재녕

전남대 화학과

An efficient palladium-catalyzed two-step protocol for the synthesis of *N*-tosyl *aza*-Baylis-Hillman adducts of acrylamide was developed. The method involved the preparation of the corresponding Baylis-Hillman adducts of acrylonitrile and the following Pd-catalyzed hydration of nitrile with acetaldoxime.

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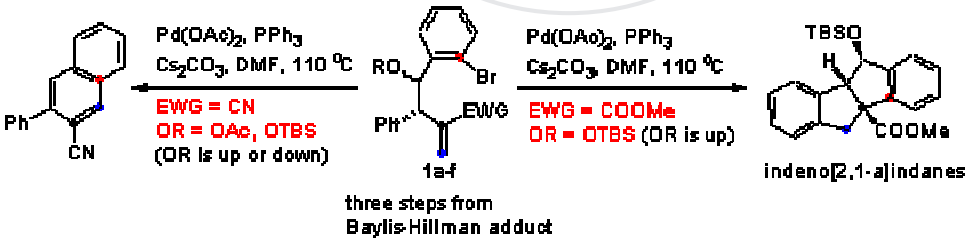
Palladium-catalyzed synthesis of indeno[2,1-a]indanes via a Heck/arylation cascade

김고훈, 김세희, 김재녕

전남대 화학과

We developed an efficient synthetic approach of novel indeno[2,1-a]indane scaffold starting from the Baylis-Hillman adduct via the combination of two key reactions: an In-mediated Barbier reaction and a Pd-catalyzed 5-*exo*-carbopalladation/arylation cascade in a highly regioselective manner (*exo/endo* > 0.91). The Pd-catalyzed cascade reactions of compounds 1a-f are highly dependent upon the protecting group of the alcohol moiety as well as EWG of the Baylis-Hillman adduct, especially in their *5-exo* versus *6-endo* carbopalladation stage. In addition, the reaction conditions, especially the kinds of a base, affect the reaction to some extent.



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발표종류: 포스터, 발표일시: 목 10:30~12:30

Mechanistic studies on the reduction of N-arylmaleimides by triphenylphosphine

이혜선, 이창규

강원대 화학과

N-(m- and p-substituted)phenylmaleimides are reduced to the corresponding succinimides by triphenylphosphine in ethanol. The side products are N-arylmaleimidic acids and N-arylsuccinimidic acids. The mechanism of the reduction has been investigated by employing various alcohols including deuterated alcohols. A possible mechanism will be discussed.

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발표종류: 포스터, 발표일시: 목 10:30~12:30

Preparation of (2E)-3-Phenyl-1-(pyrrol-3'-yl)prop-2-en-1-one

정은지, 이창규

강원대 화학과

N-Benzenesulfonylpyrrole undergoes Friedel-Crafts acylation exclusively at the 3-position of the pyrrole ring, thus allowing a simple and efficient synthesis of 3-acylated pyrroles. (2E)-3-Phenyl-1-(pyrrol-3'-yl)prop-2-en-1-one having m- and p- substituents on the benzene ring were prepared by the reactions of 3-acetyl- N-benzenesulfonylpyrrole and substituted benzaldehydes under aldol condensation conditions. 1H and 13C chemical shift values are correlated with Hammett σ values. The results are discussed.

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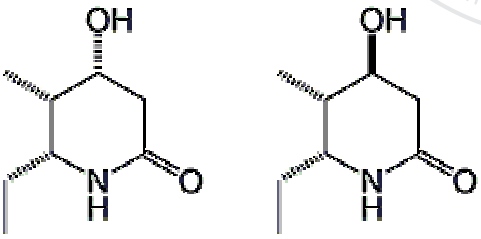
Synthesis of the lactam analogues of triketide lactones

강한영, 전기수, 오홍세

충북대 화학과

Investigations on the new analogues of existing drugs to improve their biological properties such as stability and pharmacokinetic behaviors have attracted much attention. We have studied the synthesis of macrolide antibiotics which appear in the pikromycin biosynthetic pathway. Methymycin and pikromycin families of antibiotics show activities but improvement of antimicrobial activities has been requested for these macrolide antibiotics to become competitive drugs. Developing analogues of these macrolides we became interested in synthesizing lactam analogues of these macrolides. Along this line of research, we have studies the synthesis of the lactam analogues of simple triketide lactones which we reported previously, as shown below. Synthesis of these target lactams will be presented.



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발표종류: 포스터, 발표일시: 목 10:30~12:30

Preparation of N-Aryl-3-thiophenecarboxamides and Their NMR Studies

김수진, *유지숙, 이창규

*강원대 화학과 *강원대 공동실험실습관*

3-Thiophenecarboxylic acid, which was prepared from 3-methylthiophene using sodium dichromate, was converted to anilides by treatment with thionyl chloride and subsequent reaction with m- and p-substituted anilines in the presence of triethylamine in methylene chloride. The crude anilides were recrystallized from ethanol. 1H and 13C NMR spectra of the anilides were obtained in DMSO-d6 and the chemical shift values were correlated with the Hammett σ values. All H and C chemical shifts show good positive correlation except 4-C showing only a trend and 5-C showing no correlation. But 3-C shows a negative correlation.

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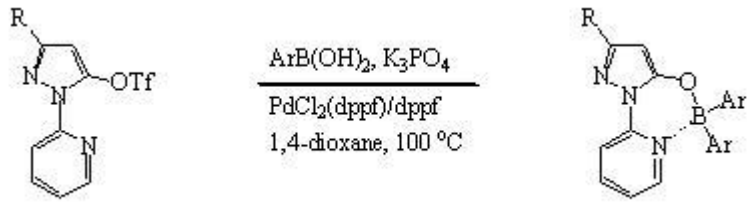
Structure determination and Identification of Diarylborinate, an unusual Suzuki product from 1-(2-pyridinyl)pyrazole with aryl boronic acid (I)

빈혜린, *서정민, **이기인

*충남대 화학과 *고려대 화학과 **한국화학연구원 신약연구단*

We have identified and determined the structure of an unusual Suzuki product, pyrazole diarylborinic acid ester, obtained from Pd-catalyzed cross-coupling of 1-(2-pyridinyl)pyrazole triflate with arylboronic acid. The reaction is not clear, however, recent results have suggested that palladium complex with Pd→B dative bond assisted by the pyridine nitrogen may favor the formation/disproportionation of diarylborinic acid/arylboronic acid.



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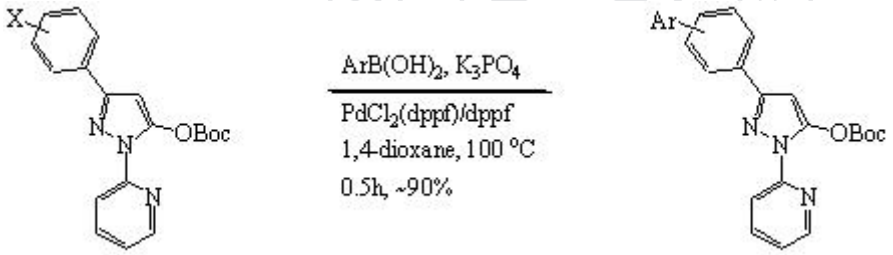
Palladium-Catalyzed arylation of enolizable 5-pyrazolone derivatives (II)

빈혜린, 김건철, *이기인

*충남대 화학과 *한국화학연구원 신약연구단*

The cross-coupling of enolizable 3-haloaryl-5-pyrazolone derivatives with arylboronic acids promoted by PdCl2(dppf) afforded 3-biarylpyrazoles in excellent yields. In this coupling, we realized that the protection of the enolizable hydroxyl group of pyrazolone is a prerequisite for ensuring the biaryl products.



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Solvent Effects on Photocyclization of 2-Hydroxy-4,6-dimethylphenacyl Benzoate

임범희, 박봉서

동국대 화학과

A mixed phenacyl photocage containing both methyl and hydroxyl group at ortho position, 2-hydroxy-4,6-dimethyl phenacyl benzoate, was prepared and its photochemical behaviors were investigated. Three different cyclization products were obtained, whose ratios varied depending on solvents. Photocyclization to the methyl side forming the indanone was a major reaction in benzene, but in protic solvents such as methanol the cyclization toward the hydroxyl group giving the coumaranone and the isocoumaranone became the predominant pathway. The product selectivity was explained by the balance between two different contribution factors of intramolecular hydrogen bond in E-dienol precursor to the indanone and in oxy-Z-dienol precursor to the coumaranone and the isocoumaranone.

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Temperature Dependent Product Selectivities in Photolysis of 2,4,6-trialkylphenacyl benzoates

류혁준, 박봉서

동국대 화학과

Photolysis of the title compound leads to two major reaction pathways: benzocyclobutenol formation from dienol intermediates resulting from photoinduced intramolecular hydrogen abstraction, and indanone formation via benzoic acid elimination from the dienol intermediates. The product ratios turn out to be dependent on the reaction temperatures. At low temperature, formation of the benzocyclobutenol is favored over the indanone. As the temperature is raised, relative amount of the indanone increases. The Arhenius plot gives ΔH and ΔS of two reaction pathways. Mechanistic implication of the results will be discussed in detail.

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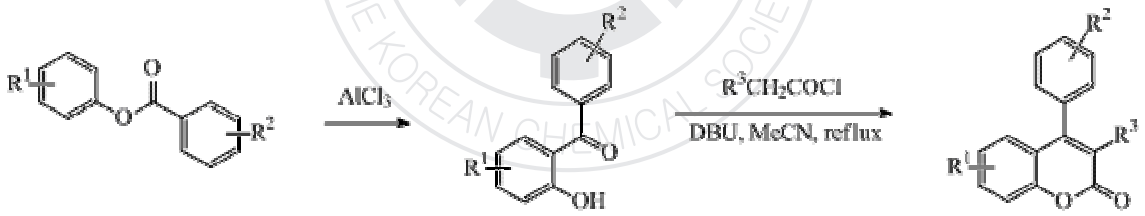
DBU-mediated synthesis of highly substituted 4-arylcoumarins from o-hydroxybenzophenones (I)

이선아, *이기인

*한국화학연구원 바이오소재연구센터 *한국화학연구원 신약연구단*

The Fries rearrangement of phenyl benzoates to the corresponding o-hydroxybenzophenones were accomplished in the presence of aluminum chloride without solvent. Highly subsitututed 4-arylcoumarins have been synthesized by the Kostanecki acylation of o-hydroxybenzophenones with acid anhydrides or acyl halides in which DBU was the best choice for the reaction.



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발표코드: **Ⅰ37P205포**
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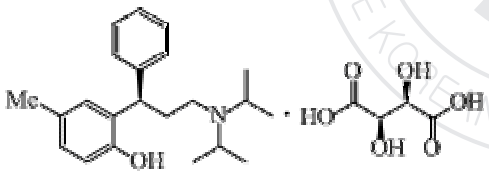
발표종류: 포스터, 발표일시: 목 10:30~12:30

A Synthetic Study toword Tolterodine Tartrate (II)

이선아, *이기인, **곽세훈

*한국화학연구원 바이오소재연구센터 *한국화학연구원 신약연구단 **과학기술연합대학원대 의약및 약품화학*

Tolterodine is a potent and competitive muscarinic receptor antagonist used in the treatment for overactive bladder disorders, including frequent urination and inability to control urination. Herein we report a practical route to tolterodine racemate with a quite straightforward manner, employing relatively cheap materials such as benzoyl chloride and acetic anhydride.



(R)-Tolterodine L-tartarate

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발표종류: 포스터, 발표일시: 목 10:30~12:30

Kinetic Studies on the Nucleophilic Substitution Reaction of 4-Chloro-7-nitrobenzofurazan with 4-X-anilines in MeOH-MeCN Mixtures.

최호준, *구인선

*경상대 화학과 *경상대 화학교육과*

The reaction rates of 4-chloro-7-nitrobenzofurazan with 4-X-anilines in methanol-acetonitrile mixtures were measured conductometry at 25 ^{o}C. It was observes that the rate constant increases in order of X = 4-OCH_3 > 4-CH_3 > H > 4-Cl. When the solvent composition was varied, the rate constant increased in order of MeOH > 50% MeOH > MeCN. The electrophilic catalysis by methanol probably consists of hydrogen bonding between alcoholic hydrogen and leaving chloride in the transition state. The nucleophilic catalysis by methanol may be ascribed to the formation of hydrogen bonds between alcoholic oxygen and hydrogens of amines in the transition state. All these results confirm that association of anilines in aprotic solvents plays an important role in defining the mechanisms of aromatic nucleophilic substitution (S_NAr).

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발표종류: 포스터, 발표일시: 목 10:30~12:30

Unusual cleavage of alkyl aryl ether linkage by hydrazine hydrate-KOH

권민진, 이창규

강원대 화학과

Reaction of 1-(p-methoxyphenyl)-4,5,6,7-tetrahydro-4-oxoindole with hydrazine hydrate in the presence of potassium hydroxide in diethylene glycol gave 1-(p-hydroxyphenyl)-4,5,6,7-tetrahydroindole in addition to the expected 1-(p-methoxyphenyl)-4,5,6,7-tetrahydroindole. The former product is a result of the cleavage of alkyl aryl ether linkage. The structure of the product was confirmed by IR and NMR spectra. Various attempts to investigate the mechanism of the cleavage of the ether linkage were carried out.

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발표종류: 포스터, 발표일시: 목 10:30~12:30

Hydride Transfer Reactions of Benzothiazolines with Acridine Compounds

한인숙, *권민진

*강원대 과학교육학부 *강원대 화학과*

Abstact The rate constants for the hydride transfer reactions of 3-substituted benzyl-2-methylbenzothiazolines, (Z-BTH: p-CH3, H, p-F, p-Cl, m-F, p-CH3, m-Cl, p-CN) with 10-benzylacridinium (bnAc+) and 10-methylacridinium (Ac+) ions have been measured spectrophotometrically in 2-propanol-H2O (4 : 1, v/v) at 25 ± 0.1 oC in order to explore the reaction mechanism. The rate constants for the hydride transfer reactions are linearly correlated with the Hammett parameters with the slope of 0.589 for Ac+ and 0.537 for bnAc+, respectively. The equilibrium constants also have been measured for the reactions of the BTH with Ac+. The BrØnsted a is less than o.5 (0.38) as we expected. This result will be discussed in terms of mechanism and compared with those of other hydride transfer reactions with NADH analogues.

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발표종류: 포스터, 발표일시: 목 10:30~12:30

A Study on the Reaction of Amines and Hypophosphorous acid with Formaldehyde

이은수, 김용환, 최순규, 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 the reaction of the aminoac

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발표종류: 포스터, 발표일시: 목 10:30~12:30

A study on the Synthesis of Di-spirohydantoins from Diaminoalkanes.

장가영, 이언진, 이용균, 정대일, *한정태, **김인식

*동아대 화학과 *영동대 뷰티케어과 **동아대병원 산업의학과*

As a part of a research program related to the synthetic study of pharmacologically interesting tropane compounds, we now report the synthesis of corrsponding novel dispirohydantoin derivatives by using di-(8-azabicyclo[3.2.1]octan-3-only)alkanes with potassium cyanide and ammonium carbonate

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발표코드: **Ⅰ37P211포**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 목 10:30~12:30

Diketone Synthesis via Pd(NHC) complex-catalyzed reaction of 4,4'-diiodobiphenyl and arylboronic acid

신은혜, 이언진, 이도훈, 최순규, 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 or ongoing studies endeavored toward wittig reaction of diketone formed by suzuki carbonylative reaction with aryl ylide to afford stilbene derivative, we report ketone synthesise via Pd(NHC) complex-catalyzed reaction of 4,4'-diiodobiphenyl , carbon monoxide (or metal carbonyl), and arylboronic acid.

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An efficient One-pot Synthesis of N-substituted Pyrroles and Nortropinones

정수경, 이언진, 이용균, 정대일, *한정태

*동아대 화학과 *영동대 뷰티케어과*

Heterocyclic moieties like pyrroles and nortropinones of biologically active synthetic and natural products. In the present study, we report a convenient one-pot synthesis of N-substituted pyrroles and nortropinones from commercially available dimethyl phosphoramidate using inorganic acid or acetone dicarboxylic acid as an effective catalyst.

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Benzyne chemistry of 2-Alkenyl- and 2-Hydrazinyl-1-Methyl pyrroles

최선영, 송주현, 송현애, 김윤영, 정대일, *한정태

*동아대 화학과 *영동대 뷰티케어과*

In recent years, the use of arynes to generate 1,2-functionalized arenes has been a growing intereat in twe field of organic synthesis.Due to its electrophilicity, a wide variety of anionic and uncharged nucleophiles readily add to arynes to generate substituted arenes.We tried the reaction of twe synthesized Michaeltype adducts and benzyne [2-(trimethylsilyl)phenyl trifluoromethanesulfonate] with CsF.

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Stereospecific Synthesis for the Sex Pheromones of Rice Leaf Folder moth. from 1,5-cyclooctadiene

김상숙, 홍용표, *최선희

*안동대 응용화학과 *(주)그린아그로텍 부설연구소*

Six sex pheromones of Rice Leaf Folder moth were stereospecifically synthesized from 1,5-cyclooctadiene. Cis-4-octene-1,8-diol derived from 1,5-cyclooctadiene was monoprotected by DHP and tosylated. Grignard reaction was twice performed for the tosylate to obtain the each pheromone

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Optical Properties of the Inclusion Complexes of a Two-photon Chromophore and Cyclodextrins

OKHIL KUMAR NAG, *우한영

*부산대 나노정보소재 *부산대 나노기술대학 나노정보소재공학과*

A two-photon (TP) fluorophore, 1,4-bis(4'-(N,N-bis(6''-(N,N,N-trimethylammonium)hexyl)amino)styryl)benzene tetrabromide (C1) and its inclusion complexes (ICs) with different type of cyclodextrins (CDs) were studied as a fluorescent tag for potential applications in multi-photon bioimaging. The linear and nonlinear optical properties of C1 in the presence of CDs were substantially modulated relative to C1 itself. TP action cross section of C1 (196 GM) was measured to be 404 GM for C1/beta-CD, 460 GM for C1/gamma-CD, and 652 GM for C1/(3 gamma : beta)-CD, (gamma-CD: beta-CD = 3:1, mole ratio). Two-photon microscopy images by using C1 and its CDs complexes as a fluorescent label suggest important molecular design guidelines for efficient TP fluorophores for biological imaging.

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Stereochemistry of the 3-azabicyclo[3.3.1]nonan-9-one derivatives by NMR spectral and single-crystal XRD studies

P. Parthiban, 박근수, 정연태

부경대 이미지시스템공학과

The widespread occurrence of 3-azabicyclo[3.3.1]nonane nucleus in various alkaloids and their diverse biological actions are the significant factors to deal with the molecules. In this study, we have synthesized a series of compounds with the 3-azabicyclo[3.3.1]nonane nucleus along with different substitutions on the bicycle. The complete 1H and 13C NMR chemical shift assignments of all the synthesized compounds were unambiguously carried out with the help of H,H-COSY/NOESY and HSQC/HMBC, respectively. Besides, the stereochemistry was unequivocally established by NOESY and H,H-COSY correlations along with the use of observed coupling constants and chemical shift/width of the ring protons. In addition, the established stereochemistry of the synthesized compounds by 1D/2D NMR studies was strengthened by single-crystal XRD analysis.

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Synthesis of Biologically Interesting Geranylated Acetophenones from Melicope Semecarpifolia

하렵개, 이용록

영남대 디스플레이화학공학부

Prenylated and geranylated acetophenones are widely distributed in nature. Interestingly, it was reported that the presence of the prenyl and geranyl group leads to remarkable increases in certain bioactivities. These groups have shown to possess many physiological properties, including anti-convulsive, antifungal, antiproliferative, and antioxidant activities. We describe a new synthetic approach for biologically interesting geranylated acetophenones. The first total syntheses of 1-(5-geranyloxy-7-hydroxy-2,2-dimethyl-2H-chromen-8-yl)ethanone and 1-[5-geranyloxy-7-hydroxy-2-methyl-2-(4-methylpent-3-enyl)-2H-chromen-8-yl]ethanone, isolated from Melicope semecarpifolia, were carried out starting from commercially available 2,4,6-trihydroxyacetophenone.

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General Methods for the Synthesis of Arylmethylene Bis(3-Hydroxy-2-Cyclohexene-1-ones) and Xanthenediones by EDDA and In(OTf)3-Catalyzed Reactions

KOLLA SRINIVASA RAO, 이용록

영남대 디스플레이화학공학부

Arylmethylene bis(3-hydroxy-2-cyclohexene-1-one) derivatives are important substrates extensively used as valuable precursors for the syntheses of xanthenes and acridinediones for laser dye technology. These compounds have also shown potent activity as antioxidants, lipoxygenase inhibitors, and a new clinical class of tyrosinase inhibitors against very important dermatological disorders including hyperpigmentation and skin melanoma. Xanthenedione derivatives have attracted considerable interest in recent years because of their important biological properties including antibacterial, antiviral, and anti-inflammatory activities, as well as positive allosteric modulators of metabotropic receptors, potent nonpeptide inhibitors of recombinant human calpain I, efficiency in photodynamic therapy, and antagonists for the paralyzing action of zoxazolamine. Efficient one-pot synthesis of arylmethylene bis(3-hydroxy-2-cyclohexene-1-ones) and xanthenediones by EDDA and In(OTf)3-catalyzed reactions was developed starting from dimedone and aryl aldehydes. The key strategies of these reactions involve domino Knoevenagel/Michael reaction or Koevenagel/Michael/Cyclodehydration reactions. The scope and limitation of the two catalysts under various reaction conditions were investigated and described.

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Efficient synthesis of biologically interesting polycycles bearing citrans and chalcones by EDDA-catalyzed reactions: Total synthesis of sumadain A and rubraine

CHEN YE, 왕설, 이용록

영남대 디스플레이화학공학부

Polycycles bearing citran or cyclol nuclei are widely distributed in nature and have a range of biological and pharmacological properties. Among these, cannabinoids containing a citran or cyclol moiety have been isolated from Cannabis sativa, also known as marijuana or hashish. An efficient and concise synthetic route for biologically interesting polycycles bearing citran and chalcone nuclei was developed starting from a variety of trihydroxybenzenes with substituents on the ring. The key strategies involved an ethylenediamine diacetate-catalyzed cyclization by a domino aldol-type/electrocyclization/H-shift/hetero Diels-Alder reaction of trihydroxybenzenes and citral or trans,trans-farnesal. This methodology was applied successfully to the synthesis of three natural products, desbenzylidenerubramin, rubraine, sumadain A and their unnatural derivatives.

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Total Synthesis of Prorepensin with a Bis-Geranylated Chalcone

TO QUANG HUY, G. SRIHARI, 이용록

영남대 디스플레이화학공학부

Geranylated chalcones are an abundant subclass of flavonoids widely distributed in nature.They have shown a variety of biological properties including antibacterial, antifungal, antitumor, antimetastatic, cancer chemopreventive, anti-HIV, anti-vasoconstriction, and antidiabetic activities and have been used in traditional medicines. The total synthesis of naturally occurring prorepensin with a bis-geranylated chalcone has been achieved by a convergent sequence. The key strategy involved in the synthesis of prorepensin was chalcone formation by aldol condensation of the corresponding geranylated acetophenone with geranylated benzaldehyde.

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Environmentally Benign Efficient One-Pot Synthesis of Spirooxindole Derivatives by EDDA-Catalyzed Reactions in Water

G. SRIHARI, 이용록

영남대 디스플레이화학공학부

Spirocyclic compounds represent an important class of naturally occurring substances with highly pronounced biological properties. Molecules bearing the spirooxindole moiety have been widely found in nature and have shown to possess a variety of important biological activities. The unique structural array and highly prominent pharmacological activities have subsequently stimulated interest in the synthesis of spirooxindole derivatives. We describe a simple and efficient one-pot synthetic approach for the preparation of biologically interesting spirooxindole derivatives using EDDA-catalyzed three component reactions of isatins, malononitrile, and 1,3-dicarbonyl compounds in an aqueous medium. This method is of great value because of its environmentally benign character, high yield, and easy handling.

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Iodine-Catalyzed One-Pot Synthesis of 2H-Pyrans

LI XIN, 정은진, 이용록

영남대 디스플레이화학공학부

2H-Pyrans are important core units in a number of natural products and also in photochromic materials.The molecules bearing 2H-pyrans have a variety of interesting biological activities and potential medical applications. We have been developed the methodologies for the synthesis of 2H-pyrans through indium(III) chloride- or EDDA-catalyzed formal [3+3] cycloaddition as a Lewis acid or a Brønsted acid and base catalyst. Later, novel approaches for the synthesis of 2H-pyrans were also developed by other groups using BF3-Et2O, TiCl4, and In(OTf)3 Lewis acids as a catalyst and phosphoric acid as a Brønsted acid catalyst. Although several synthetic approaches for constructing 2H-pyrans derivatives have been reported by us and other groups, more simple and cost-effective approaches are still demand because of their imporatance. A facile and efficient synthesis of 2H-pyrans is achieved by iodine-catalyzed reactions of 1,3-dicarbonyl compounds with a variety of α, β-unsaturated aldehydes in moderate yields. The key strategy is a formal [3+3] cycloaddition by domino Knoevenagel/electrocylization. This method has been applied to the synthesis of naturally occurring pyranoquinolinone alkaloids.

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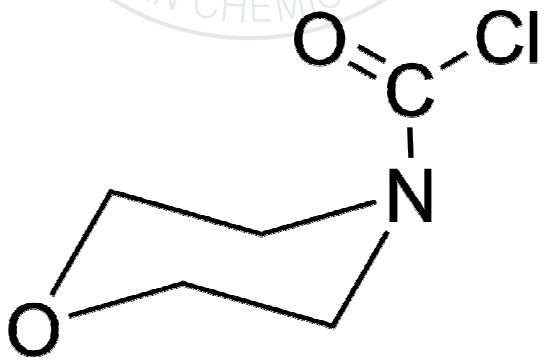
Correlation of the Rates of Solvolysis of 4-Morpholinecarbonyl chlorideUsing the Extended Grunwald-Winstein Equation

김란, *최호준, 양기열, 구인선

*경상대 화학교육과 *경상대 화학과*

We determined rate constants for solvolyses of 4-morpholinecarbonyl chloride (MPC) in aqueous binary solvents of acetone, ethanol, methanol, methanol-d, trifluoroethanol (TFE), pure water, and D_2O at various temperatures. Mechanistic variation and/or transition state variation are also discussed by applying the Grunwald-Winstein equation, extended Grunwald-Winstein equation, Z values, kinetic solvent isotope effects (KSIE) and activation parameters. In extending this work to the reactions of carbonyl chloride, we examined solvolyses of MPC with *N*-alkyl group and found that these also showed competing reaction channels.



morpholinecarbonyl chloride (MPC)

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Heteroleptic Cyclometalated Ir(Ⅲ) complexes with Highly efficient

강현주, 이금희, 윤승수, *김영관

*성균관대 화학과 *홍익대 기초과학과*

Organic light-emitting diodes (OLEDs) based on phosphorescent materials have significantly improved electroluminescence (EL) performance because both single and triplet excitons can be harvested for light emission. In principle, Phosphorescent OLEDs are possible to increase their internal quantum efficiency to 100 %, corresponding to an external quantum efficiency of more than 20 %.In this paper, a new series of heteroleptic cyclometalated iridium complexes with various aromatic systems were synthesized and their photophysical properties were investigated. Multilayered, organic light-emitting diodes (OLEDs) were fabricated to explore the electroluminescent properties of these materials by employing the complexes as dopant. This study revealed that these new iridium complexes had highly efficient electroluminescent properties.

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Naked Eye Sensing of Silver Ion Using Charge-Transfer Interaction

이재욱, 김성민, 한승철

동아대 화학과

Donor–acceptor interactions or charge transfer (CT) interactions are an important class of non-covalent interactions and have been widely exploited in self-assembling systems. Here we report the host induced intramolecular CT complex formation between the electron-rich and electron-deficient units of a single guest molecule. Through this intramolecular CT interaction, we will discuss for sensing of sliver cation by the observation of color change.

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Convergent Synthesis of Symmetrical Denderimers via Double Click of the Fréchet-type Dendrons

이재욱, 박다정, 한승철

동아대 화학과

The well-known click chemistry which is useful tool for synthesis of dendrimers, is a Cu(I)-catalyzed azide-alkyne [3 + 2] cycloaddition proved to be an ideal reaction in very good to excellent yields. Staudinger/aza-Wittig reactions (new click reaction) between azide and aldehyde are a powerful tool in organic synthetic strategies directed towards the construction of nitrogen-containing compounds. Taking advantage of these facts, herein we will use the first click reaction (Staudinger/aza-Wittig reaction) leading to the alkyne-functionalized Fréchet monodendrons containing the benzene at a core, and then will use the second click reaction (1,3-dipolar cycloaddition reaction) with azide-dendrons leading to the formation of symmetrical Fréchet-type dendrimers.

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Convergent Synthesis of Unsymmetrical Diblock Denderimers via Double Click of the Fréchet-type Dendrons with 1,4-Bis-Azidomethyl-Benzene

이재욱, 지원호, 한승철

동아대 화학과

Recently, Tornøe and Sharpless independently reported a copper(I)-catalyzed Huisgen [2 + 3] dipolar cycloaddition reaction between an terminal alkyne and an organic azide in which the 1,4-regioisomer is exclusively formed and which also allows the rapid synthesis of compound libraries. This 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. Taking advantage of these facts, herein we present the efficient strategy for the convergent synthesis of unsymmetrical diblock dendrimers containing the benzene at a core via double click reaction.

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Synthesis and Characterization of the Fréchet-type Dendrimers Containing Carbazole as a Chromophore Core

이재욱, 송태규, 한승철

동아대 화학과

The synthetic strategy for the convergent synthesis of emissive Fréchet-type dendrimers having the carbazole unit at a core via the copper-catalyzed 1,3-dipolar cycloaddition reaction between alkyne and azide will be disclosed. 3,6-Diazido-9-octyl-8H-carbazole, designed and synthesized to serve as the core in dendrimer, was stitched with the propargyl-functionalized Fréchet-type dendrons by the click chemistry, high yield and easy to isolation, leading to the formation of fluorescent Fréchet-type dendrimers.

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Synthesis of Tailor-Made Nano-Porous Polyaniline derived with PVA Stabilizer/Alkaline Metals and its Complexation with Chromium Ion

이찬우, *송영호, *최상협, *윤구식, *지기환

*울산대 화학 *울산대 화학과*

Nano-porous polyanilines (PANI) have attracted attention because of well-defined molecule structures and chemical versatility, which also complicate the mechanism of interactions between metal ions and PANI. To further understand the complexation with metal ions, tailor-made nano-porous PANIs were synthesized by self-stabilized dispersion polymerization (SSDP) method using poly(vinyl alcohol) (PVA) stabilizer/alkaline metal.This tailor-made PANI-emeraldine base (EB) was easily oxidized by a Cr(VI) oxidant $K_2Cr_2O_7$ based on the unique redox properties of PANI resulting in an oxidized form of PANI with a rigid polymer template and effective metal ion binding sites. The effective adsorption results for removal of Cr(III) ions in aqueous solution were obtained by the nano-porus PANI derived from PVA/Li system. More detail on this phenomenon will be discussed in this poster.

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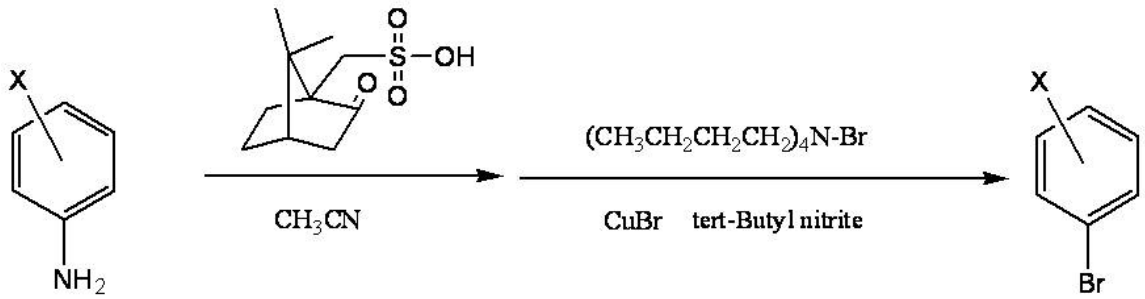
Bromination of Primary Aromatic Amines with 10-Camphorsulfonic Acid in Solvent and Solvent-Free Condition

문미은, 지기환

울산대 화학과

Aromatic diazonium salts have been used as an important building block in modern as well as classical organic synthesis. Previously we had showed bromination and chlorination of aryl amines by the facile and safety methodology via aryl diazonium tosylate salts. Recently we have developed easy one-pot synthetic method for the bromination of primary aromatic amines with 10-camphorsulfonic acid. Also the reactions were carried out in solvent-free condition. The good results by the eco-friendly methodologies will be showed and discussed in this poster.



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발표종류: 포스터, 발표일시: 목 10:30~12:30

Discrete Supramolecular Architecture Composed of Flexible Pyridine-4-carbaldehyde Azine and a 120° Pt Acceptor

VERMA SHASHI, 문미은, 지기환

울산대 화학과

The interaction of predesigned 120° Pt(II) molecular clip with flexible pyridine-4-carbaldehyde azine in 1:1 molar ratio in acetone leads to the formation of discrete self-assembly in a high yield. Characterization of the supermolecule by multinuclear ^{31}P and ^{1}H NMR spectroscopies, elemental analysis and electrospray mass spectrometry is also reported.

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Self-Assembly of Molecular Triangle via Pyridine-4-Carbaldehyde Azine and a 90° Pt Acceptor

VERMA SHASHI, 최영화, 김인수, 지기환

울산대 화학과

Pt(II) supermolecule was self-assembled by organoplatinum 90° acceptor unit and a flexible N donor ligand. It was prepared in essentially quantitative yield via spontaneous self-assembly of preprogrammed angular unit and pyridine-4-carbaldehyde azine in 1:1 molar ratio in nitromethane at room temperature. Characterization was accomplished with multinuclear NMR, ESI mass spectral data and elemental analysis. Final structure has been established on the basis of X-ray crystallography.

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Pd acceptor and Pt donor based Self-assembly:Synthesis and Characterization

vajpayee vaishali, *Stang P. J., 김인수, 지기환

*울산대 화학과 *University Of Utah*

Self-assembly is an autonomous organization of components into stable, structurally well defined aggregates without human intervention. The power and beauty of spontaneous self-assembly derives from its ability to rapidly, and simply, generate large, complex, and sophisticated “supermolecules” from easily available building blocks with maximum efficiency, generally under mild conditions. Herein, we wish to present the new heterometallic self-assembled derivatives of Pd and Pt. The newly synthesized derivative was characterized by UV, IR, NMR studies and the heterometallic square was confirmed by x-ray crystallography.

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Tetra- and Hexa-nuclear p-Cymeneruthenium Complexes via Self-Assembly and their Characterization

vajpayee vaishali, 박주연, *Stang P. J., 지기환

*울산대 화학과 *University of Utah*

The metal-mediated rational construction of discrete molecular assemblies is one of the thriving areas of supramolecular chemistry. Many examples of structurally fascinating compounds have been designed and prepared according to this synthetic paradigm, and some of them are finding applications as receptors and molecular vessels for trapping reactive intermediates and for stoichiometric and catalytic reactions. So far a multitude of two- and three-dimensional structures incorporating transition metals with square-planar geometry have been synthesized. In the search for new building blocks for the synthesis of supramolecular materials with interesting properties, there is an increasing interest in using transition metal complexes with octahedral geometry. To exploit this chemistry, we attempted for the synthesis of p-cymeneruthenium complexes with some di- or tri-pyridyl organic donors and these newly synthesized derivatives were characterized by UV, NMR spectroscopy and x-ray crystallography.

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Novel C-Aryl Glucoside SGLT2 Inhibitors as Potential Antidiabetic Agents: Pyridazinylmethylphenyl Glucoside Congeners

김민주, 이준원, 강석연, 이석호, 송광섭, *김정민, 이진화

*(주)녹십자 종합연구소/의학화학팀 *(주)녹십자 종합연구소/신약개발팀*

Dapagliflozin (Bristol-Myers Squibb/AstraZeneca) is a potential first-in-class inhibitor of sodium-glucose cotransporter2 (SGLT2) for the treatment of type 2 diabetes. Currently, only one other SGLT2 inhibitor is in Phase III clinical development-canagliflozin (Mitsubishi Tanabe Pharm/Johnson & Johnson)-for which a Phase III trial in type 2 diabetes started in August 2009. In the present study, metabolically more stable C-glucosides bearing a heteroaromatic ring were exploited in order to develop novel SGLT2 targeting antidiabetic agents. We envisioned that replacement of the distal ring of dapagliflozin with a heterocyclic ring was a worthy approach for the improvement of the partition coefficient (logP) value, to potentially decrease plasma protein binding. For this purpose, among a variety of heterocycles, we decided to screen pyridazine as our current efforts. Herein, we report the design, synthesis and biological evaluation of pyridazinylmethylphenyl glucoside congeners.

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Synthesis of novel C-glucosides with 1,3,4-thiadiazole ring as sodium-dependent glucose cotransporter 2 inhibitor for the treatment of type 2 diabetes mellitus

이준원, 서희정, 이석호, 김정민, *강재효, 이진화

*(주)녹십자 종합연구소 *서강대 화학과*

Novel C-glucosides bearing 1,3,4-thiadiazole ring at distal ring position were investigated in order to develop sodium-dependent glucose cotransporter 2 (SGLT2) targeting antidiabetic agents. A variety of derivatives containing 1,3,4-thiadiazole moieties were designed and efficiently synthesized. Several derivatives were identified as potent inhibitors for SGLT2 (IC50 < 10 nM). A selected promising compound demonstrated reasonable urinary glucose excretion in normal SD rats along with favorable blood glucose-lowering effects in db/db mice. The information obtained from the SAR studies in this study might help to design more active SGLT2 inhibitors that are structurally related.

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A Carbonate compound with the Fluorenyl Spiro Framework

심윤수, *박은묵, *나춘섭, **박규순

*영남대 이과대 화학과 *영남대 화학과 **국민대 화학과*

A five-membered cyclic carbonate with a fluorenyl spiro framework was prepared by coupling of the corresponding epoxide with carbon dioxide in the presence of catalytic amount of quaternary ammonium salts in a high yield. Efficiency and activity profiles of quaternary salts for this reaction were described

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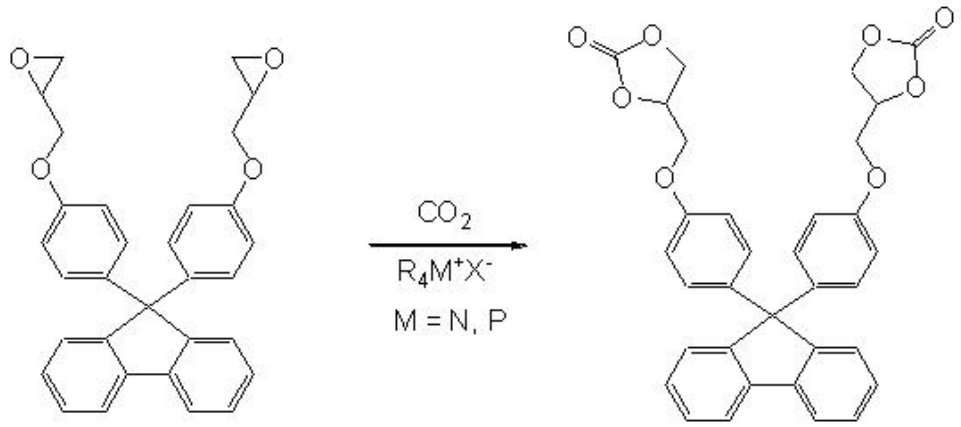
CO2
R4M+X-
M = N, P

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Expeditious synthesis of highly substituted indolizinones via palladium-catalyzed tandem sequence

김경선, 최기항, *김익연

*고려대 화학과 *한국화학연구원 의약화학연구센터*

Described herein is a direct one-pot route to poly-substituted indolizinones from tertiary propargylic alcohols using palladium-catalyzed tandem process involving aminopalladation, 1,2-shift, and reductive elimation.

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Lipoic acid and polyphenolic hybrid molecules for cholinesterase inhibitor

우연지, *연고흠, 이보현, 김현주, **이봉호, **고장면, **박정호

*한밭대 응용화학생명공학과 *한밭대 응용화학과 **한밭대 응용화학생명공학부*

Although oxidation reactions are crucial for life, they can also be damaging; consequently, body maintains complex systems of multiple types of antioxidants, such as vitamin C, vitamin E, polyphenols and lipoic acid.In this study, we have synthesized a series of lipoic acid - polyphenol derivative through amines linker. And the biological activities such as antioxidant activity and anticholinesterase inhibitory activities are measured.

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Functionalized Synthesis of Various Organotrifluoroborates for Suzuki-Myaura Cross-Coupling Reaction Partners

김동수, 전상일, *함정엽

*강릉대 화학과 *KIST 천연물소재연구센터*

Potassium organotrifluoroborate 는 수분과 공기중에서 안정한 결정형 고체 화합물로 Suzuki-Myaura Cross-Coupling reaction 에 중간체로 사용되는 중요한 coupling partner 이다. 하지만 이러한 장점에도 불구하고, 공기중에 불안정하고, 값비싼 또다른 coupling partner 인 boronic acid 와 boronate ester 류 화합물이 상업적으로 구입 가능하고, 많이 쓰이고 있는 실정이다. 이와 같은 이유로 다양하게 functionalized 된 novel 하고 unique 한 Potassium organotrifluoroborate 유도체의 개발이 절실히 요구되어 왔다. 최근 본 연구진은, alkynylaryl 기능기를 가지는 potassium alkynylaryltrifluoroborate 의 개발에 성공하여 이를 이용한 microwave-promoted Suzuki-Myaura Cross-Coupling reaction 을 성공적으로 수행하였고, 더 나아가 Jones oxidation 을 이용해 자체 개발한 potassium hydroxyltrifluoroborate 를 aldehyde 또는 ketone 으로 변환하는 연구를 활발히 진행중에 있다.

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Synthesis and electrochemical properties of azo and anthraquinone derivatives

정지윤, 박종욱, 박영일

가톨릭대 화학과

For full color realization of liquid crystal display (LCD), a color filter (CF) is necessary to change white back light into red (R), green (G) and blue (B) lights. In such CF, black matrix (BM) materials are between each R, G, B color pixels for high contrast. Although Cr/CrOx with sputtering process has been in use as BM, Cr is a heavy metal element that causes environmental problems itself. And high cost and complicated sputtering process are increasing the necessity of an organic BM material. Among new BM materials, it is very important to develop black pigment which is the core material of organic BM. 1-(4-Phenylazo-naphthalen-1-ylamino)-anthraquinone (AAQ), and 1,4-Bis-(4-phenylazo-naphthalen-1-ylamino)-anthraquinone (DAAQ) were synthesized. UV-visible spectra of the synthesized AAQ and DAAQ showed UV_{max} values at 428 and 481 nm. In the case of DAAQ, it was found that the entire range of visible light wavelengths 400-800nm are absorbed. In addition, as a result of measuring PL spectra of the synthesized materials, both materials did not show PL spectra. The electrochemical kinetic properties of the synthesized materials were evaluated via CV at various scan rates 30 mV/s ~ 150 mV/s. As a result, exponent values of scan rate for AAQ and DAAQ were 0.38 and 0.42 and both did not reach diffusion control process. Their electron active speeds were not fast but both materials showed high thermal stability as T_d of 353 and 366℃.

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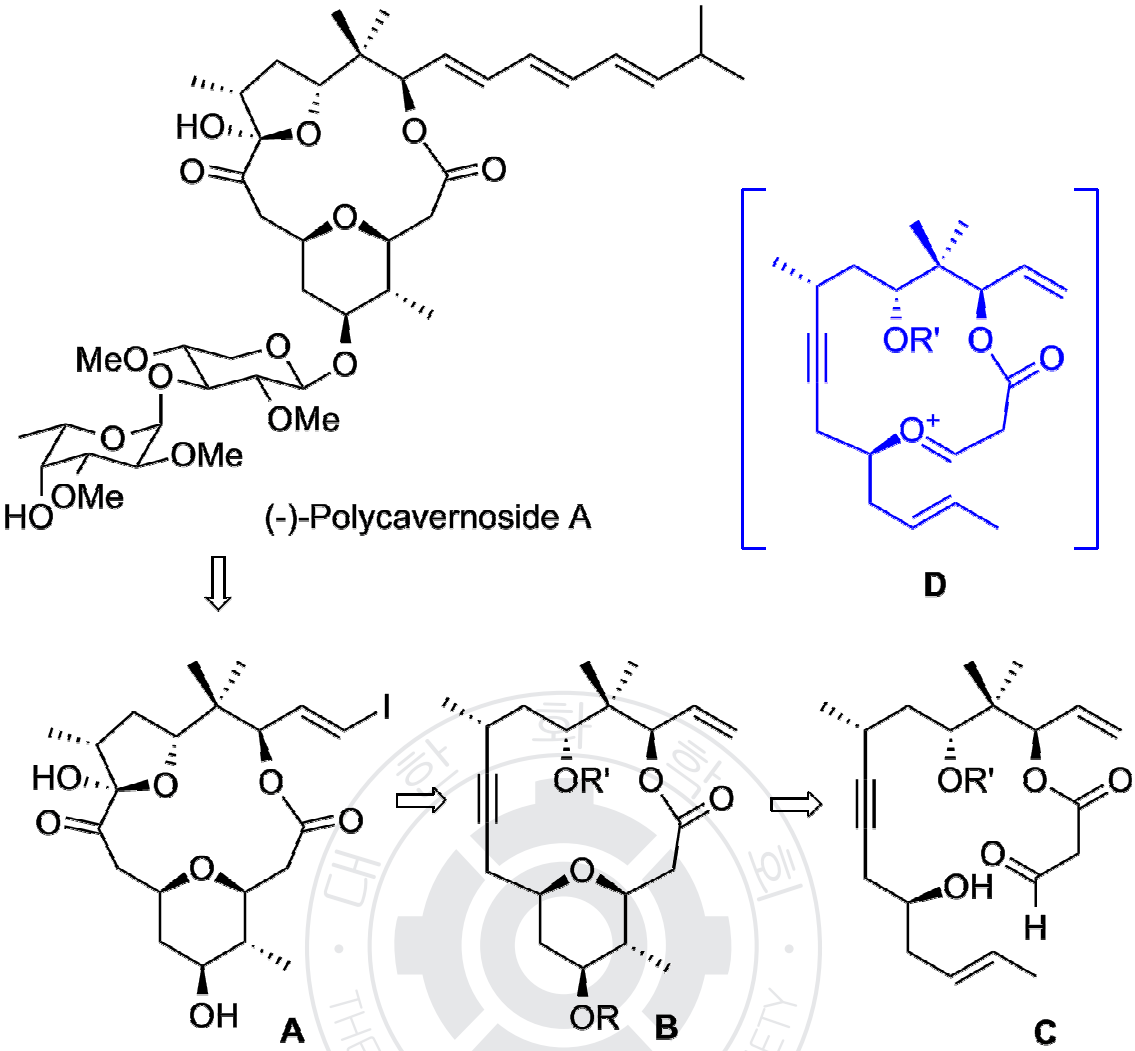
Polycavernoside A: The Prins Macrocyclization Approach

우상국, 이은

서울대 화학부

Polycavernoside A was isolated by Yasumoto from the edible red alga *Polycavernosa tsudai* as a causative toxin of sudden human intoxication in Guam in 1991. The proposed macrolactone disaccharide structure was confirmed via the first total synthesis of Murai, which also established the absolute stereochemistry. We were intrigued by the possibility of using intramolecular Prins macrocyclization protocol in the synthesis of polycavernoside A. Aldehydo homoallylic alcohol C may undergo Prins cycllization reaction to produce macrolactone B, from which the known macrolactone intermediate A may be prepared. The success of this macrobicyclization reaction hinges on the viability of the macrocyclic oxocarbenium ion D.


HO
O
O
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O
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MeO
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OMe
O
OMe
HO
OMe
(-)-Polycavernoside A
OR'
O
O
O+
D
I
HO
O
O
O
O
OH
A
OR'
O
O
O
OR
B
OR'
O
O
O
OH
H
C

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Synthesis and Electrochemical Properties of Bis(dipyrrinato)zinc Complex Derivatives

이소라, 박영일, 박종욱

가톨릭대 화학과

1- and 2- positioned of naphthalene group were substituted into 5- position of dipyrrinato with the use of bis(dipyrrinato)zinc complex moiety, and bis[5-(1-naphthalenyl)-dipyrrinato]zinc complex ($Zn(1\text{-}NaPN)_2$) and bis[5-(2-naphthalenyl)-dipyrrinato]zinc complex ($Zn(2\text{-}NaPN)_2$) , which are the derivatives of bis(dipyrrinato)zinc complex, were successfully synthesized. The optical properties of the synthesized compounds were measured through UV-visible and PL spectrum. The UV-visible maximum values in solution state, 485 and 486 nm for $Zn(1\text{-}NaPN)_2$ and $Zn(2\text{-}NaPN)_2$ respectively, have similar absorption maximum value. PL spectrum maximum values, 516 and 518 nm. In the film state, UV-visible maximum values, about 517 nm for both substances, indicated absorption of similar wavelengths. PL spectrum was shown to be about 550 nm which is also red-shifted about 33 nm from the solution state, moving toward yellowish green color.$Zn(1\text{-}NaPN)_2$ and $Zn(2\text{-}NaPN)_2$, the synthesized compounds, were measured on electrochemical kinetic properties through cyclic voltammogram (CV), and both materials showed similar oxidation voltage of about 0.7 V (vs. $Ag/AgNO_3$). The exponent of scan rate and x value of $Zn(1\text{-}NaPN)_2$ and $Zn(2\text{-}NaPN)_2$ were 0.52 and 0.33, so the kinetics of $Zn(1\text{-}NaPN)_2$ is mainly controlled by diffusion process.

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Preparation of PAMAM Dendrimer-Organosilane Hybrid

최고은, 신은주, *고희찬

*순천대 화학과 *(주)코일렉트로드 연구부*

Polymer-organosilane hybrid materials were extensively studied because of improvement of surface properties for hybrid coating. However, use of dendrimer in place of polymer was reported scarcely. A variety of dendrimers have been studied for their structural uniqueness to allow feasible molecular design and well-defined array. For obtaining the properties of good corrosion-resistance, abrasion-resistance, heat-resistance, hardness, adherence to metal surface, transparency, and less cracking, dendrimer-organosilane hybrids were prepared from amino-terminated poly(amidoamine) generation 3 and tetraethoxysilane and 3-glycidoxypropyltrimethoxysilane by in situ sol-gel process. Optical microscope image showed that these transparent hybrids have the nanocomposite structure. Their structural properties were characterized by ultraviolet spectra and infrared spectra. Surface properties of coating on steel and glass using this hybrid were determined by pencil hardness tester.

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Preparation of Zinc Porphyrin-Pyridine Dendrimer via Axial Coordination

최고은, 신은주

순천대 화학과

Porphyrin is not only a well-known luminescent and redox active compound that can accomplish the photoinduced electron transfer in photosynthetic reaction center, but also is frequently observed in porphyrin-containing enzyme manifesting the enzyme activity by carrying out the axial coordination on central metal of metalloporphyrin plane. A variety of dendrimers have been studied for their structural uniqueness to allow feasible molecular design and well-defined array. This study deals with how the dendritic environments of pyridine-containing dendrimers affect the axial coordination of pyridine-containing dendrimers on zinc porphyrin as a model of high dimensional porphyrin dendrimer.

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Photochromic Behavior of Zinc Porphyrin- Spiropyran Dyad

박태종, 신은주

순천대 화학과

Metalloporphyrin is a key compound for light energy harvesting and long-range electron transfer to reaction center in plants and photosynthetic bacteria. Zinc porphyrin is one of most frequently employed photoactive molecules due to its spectral and redox properties. Numerous research groups have designed and prepared the molecular energy storage devices containing porphyrin moiety. Spiropyran is well-known photochromic compound accomplishing molecular structural change to merocyanine form by ring opening on UV irradiation. In turn, merocyanine is transformed to spiropyran by ring closure on irradiation of visible light Reversible photochromic spiropyran-merocyanine transformation is one of the subject of active research on optical memory and switch. Incorporating photochromic molecules into organic materials leads to photoresponsive systems, the properties of which can be manipulated by light. 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. In this study, Zinc porphyrin-spiropyran dyad was prepared and the photochromic behavior was investigated.

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Preparation of Spiropyran-Organosilane Hybrid

박태종, 신은주, *고희찬

*순천대 화학과 *(주)코일렉트로드 연구부*

Organic-inorganic hybrid coating is most promising anti-corrosion material for protecting various metal surfaces. Organic materials are more tough, flexible, and processable, while inorganic materials are more heat-resistant, mechanically strong, hard, and less abrasive. Organic-inorganic hybrid materials by combination of organic and inorganic materials have been investigated to get the advantages of both two materials. Using sol-gel method for preparing inorganic polymer at low temperature, organic-inorganic hybrid could be prepared. Spiropyran is well-known photochromic compound accomplishing molecular structural change to merocyanine form by ring opening on UV irradiation. In turn, merocyanine is transformed to spiropyran by ring closure on irradiation of visible light Reversible photochromic spiropyran-merocyanine transformation is one of the subject of active research on optical memory and switch. In this study, spiropyran-organosilane dyad was prepared and the photochromic behavior was investigated.

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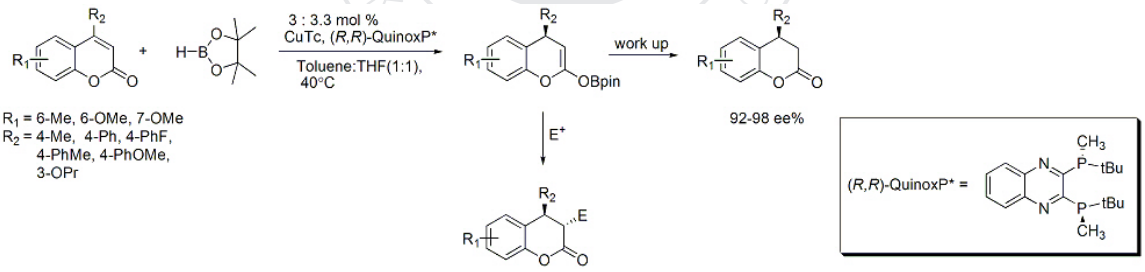
Copper-Catalyzed Asymmetric Conjugate Reductions of Coumarins with Pinacolborane(PinBH)

김효현, 윤재숙

성균관대 화학과

Coumarin derivatives are important in a number of physiologically active compounds. We have developed an efficient enantioselective conjugate reduction of coumarins with copper(I)-QuinoxP* catalyst in the presence of pinacolborane(PinBH) as the stoichiometric reducing agent. We successfully reduced coumarins in high yields with excellent enantioselectivity (up to 98% ee) and developed a catalytic enantioselective aldol reaction with aldehydes or ketones.



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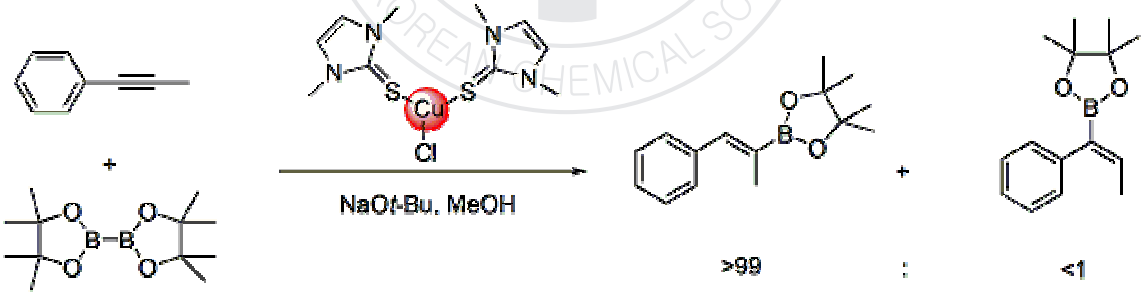
Bis(imidazoline-2-thione)-copper(I)catalyzed regioselective borylation of internal alkynes

김혜령, 윤재숙

성균관대 화학과

Boration of alkynes is a useful method for the preparation of alkenyl boranes, versatile organic building blocks with use in subsequent couplings. The transition metal catalyzed hydroboration of internal alkyne with hydroboranes generates the syn-adductive product, but a significant regioselectivity problem arises. We report efficient copper systems that regioselectively afford hydroborated products from internal alkynes with use of diboron reagent using imidazoline-2-thiones as new ligand.



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Syntheses and Chemical Properties of π-Extended Sapphyrin, Rosarin and Rubyrin

이창희, 유수연, 김수진

강원대 화학과

1,10-Dihydrobenzo[e]pyrrolo[3,2-g]indole (naphthobipyrrole) and its derivatives was synthsized as a building block for the synthesis of pi-extended, expanded porphyrins. The utility of the synthesized building block has been demonstrated by synthesizing several new porphyrinoid macrocycles including naphthorosarin, naphthorubyrin and naphthosapphyrin. The naphthorosarin was synthesized by acid-catalyzed condensation of naphthobipyrrole and pentafluorobenzaldehyde. The naphthorubyrin and naphthosapphyrin were synthesized by three component condensation including naphthobipyrrole, pentafluorobenzaldehyde and pyrrrole. The structure of the naphthorosarin and naphthorubyrin were determined by 1H NMR, 13C NMR, HRMS and single crystal X-ray diffraction. In the case of naphthorosarin, the planar geometry and the existence of three pyrrole N-Hs in the core was confirmed by low temperature 1H NMR spectroscopy. Although the signal of the pyrrole N-Hs was appeared at 3.5 ppm suggesting some aromatic character, the system seems to contain 24-pi, that indicative of anti-aromatic character. Naphthorubyrin, on the other hand, was basic and the isolated compound was mono-protonated form. Large hypsochromic shift of Q-bands was observed on protonatio/deprotonation. Naphthosapphyrin exhibited full aromatic character with one inverted pyrrole ring. The re-inversion of the inverted pyrrole was observed upon treatment with acid.

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Synthesis and Anion Recognition Properties of Pyrrole-Strapped Calix[4]pyrroles

이창희, 박건유, 엄가영

강원대 화학과

Calix[4]pyrroles have been studied as novel neutral anion-binding receptor since the anion-binding property was discovered in 1996. Various modifications have been attempted in conjunction with improving the binding properties. We have synthesized few pyrrole-strapped calix[4]pyrroles bearing signaling unit at the beta-pyrrolic positions. The synthesis was accomplished by Sonogashira coupling of iodo-pyrrole and various fluorophores including pyrenes and BODPY. The identity of the products was fully characterized by spectroscopic means including proton NMR, HRMS and single crystal X-ray crystalography. The binding studies indicate that the titled receptor could be excellent fluorogenic anion receptors for fluoride anion. The anion selectivity and binding affinity will be presented.

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Ion-Selective Recognition of Calix[4]pyrrole-Based Ion-Pair Receptors

이창희, 김보향, 이유림

강원대 화학과

We designed and synthesized the ditopic ion-pair receptors based on the caix[4]pyrroles, oligoethylene glycol and calix[4]crown. The synthesis of the calix[4]pyrroles bearing a diametrically crossing tetra- or penta-ethylene glycol strap was accomplished by condensation of oligoether podand-like bis-dipyrromethanes with acetone in the presence of acid catalyst. The calix[4]pyrrole diametrically connected with m-dibenzo-[26]-crown-8 was also synthesized and fully characterized in order to improve the ion-pair binding selectivity. The structure was characterized by 1H NMR, 13C NMR, MALDI-TOF MS as well as single crystal X-ray crystalography. 1H NMR spectroscopic analyses confirm that the titled receptors forms strong 1:1 complex with fluoride anion. The bound fluoride anion was easily decomplexed upon treatment with Na+ or Li+ cation. On the other hand, the fluoride-bound host forms strong ion-pair complex with Cs+ cation. The Cs+ bound to the cup of calix[4]pyrrole generated by conformational change upon fluoride binding. In the case of chloride complex, only Li+ cation bound to the oligoether moiety to form a tight ion-pair. The Cs+ binds to the cup of calix[4]pyrrole and partial decomplexation was observed with Na+ and K+.

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Pyrene Incorporated Calix[4]pyrroles: Synthesis and Molecular Recognition

이창희, 박경화, 유재덕

강원대 화학과

We have synthesized several new calix[4]pyrroles that bear fluorogenic pyrene as a part of the macrocycle. The synthesized compounds were characterized by proton NMR, HRMS and single crystal X-ray crystalography. The most of the compounds show excellent affinity toward anionic guests as well as some neutral molecules including C60 and polynitroaromatics. Especially, excellent binding affinity was observed to fullerenes with the detection limit of nano-molar range. The emission spectra are dramatically changing depending on the solvent. Monomeric pyrene emission is observed in toluene and pure excimer emission is observed in acetonitrile on the other hand. The detailed binding studies with various guest molecules as well as fluorescence properties will be presented.

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Dicyanovinyl Substituted, Strapped Calix[4]pyrrole as a Novel Cyanide-Selective Ratiometric Chemosensors

이창희, 홍성진, 이혜영

강원대 화학과

Isophthalate-strapped calix[4]pyrrole which is originally transparent in visible region, becomes colored (λmax =403 nm in acetonitrile) by introduction of dicyanovinyl group at beta-pyrrolic position. The synthesized host molecule form stable complex with various anions with hypsochromic shift of the absorption spectra. When the host is titrated with cyanide anion, complete bleaching of the colour is observed. The spectroscopic evidences indicate that the cyanide is added to the alpha-position of dicyanovinyl group forming a ketimine. The compound is a dual functional, chemodosimeteric sensor model and found to react selectively with cyanide anion. The rate of bleaching becomes faster when other anions are co-present. Anion-binding affinities were measured and the value is compared with those of other beta-vinyl substituted calix[4]pyrroles. The receptors that bear both anion binding site and electrophilic addition site could be beneficial achieving higher anion selectivity and reducing inhibitory effect from other anions.

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Calix[4]pyrrole-Based Fluorescence 'TURN-ON' Probes for Anionic Guests

이창희, Punidha Sokkalingam

강원대 화학과

We designed and demonstrated anionic fluorophore-bound calix[4]pyrrole that can sense fluoride anions in micromolar concentration. When the highly fluorescent fluorophore, 4-trifluoromethyl-7-hydroxycoumarate, is bound to the calix[4]pyrrole core through hydrogen bonding, the fluorescence of the coumrate is completely quenched. However, the fluorescence was gradually recovered upon titration with anionic guests like fluoride. Since fluoride anion has stronger affinity to calixpyrrole as compared with coumarate anion, the coumarate anion is replaced with fluoride anion. As a result, now these free coumarates have regained its fluorescence properties. The increase in the fluorescence intensity was found to be closely related with the concentration of released coumarate anion. Since all the anionic guests have different affinity with calix[4]pyrrole, the linear relationship between anionic guests and regained fluorescence intensity is expected. Indeed, this is the case and good correlation between anion concentration and fluorescence intensity was observed.

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Synthesis and Chemical Properties of Expanded meso-Alkylidenyl Porphyrinoids

이창희, 정승두, 박자영, *김한제

*강원대 화학과 *공주교육대 초등과학교육과*

The synthesis and characterization of meso-Alkylidenyl expanded porphyrinoid macrocycles and their Schiff-base analogs will be described. The synthesis of these substances, which all contain unique exocyclic C-C double bonds at multiple meso-positions, are 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 of the synthesized compounds. The Schiff-base macrocycles are somewhat resistant to the DDQ-oxidation and resulted in the formation of macrocyclic imines bearing sp3-hybridized meso-carbons.

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Synthesis of Chalcone Derivatives and Comparison of their Antioxidant Effects

김미란, 전종갑

한림대 화학과

Flavonoid 계통의 화합물인 chalcone 은 혈압강하, 혈당조절, 항염증 작용과 최근 주목 받고 있는 항산화효과등의 생리활성을 갖는다고 알려져 있다. Chalcone 화합물은 A ring 의 catechol 구조와 B ring 의 resosinol 구조를 갖는 화합물이 뛰어난 항산화 효과를 나타낸다고 알려져 있다. 이러한 구조적인 특징을 확인하기 위하여 치환기의 위치를 바꾸어 보았다. Base 조건과 acid 조건에서 Aldol condensation 으로 chalcone 화합물을 합성하였고, 합성된 화학물의 항산화력을 DPPH, ABTS 그리고 tyrosinase enzyme 을 이용하여 radical scavenging 효과를 비교하였다.

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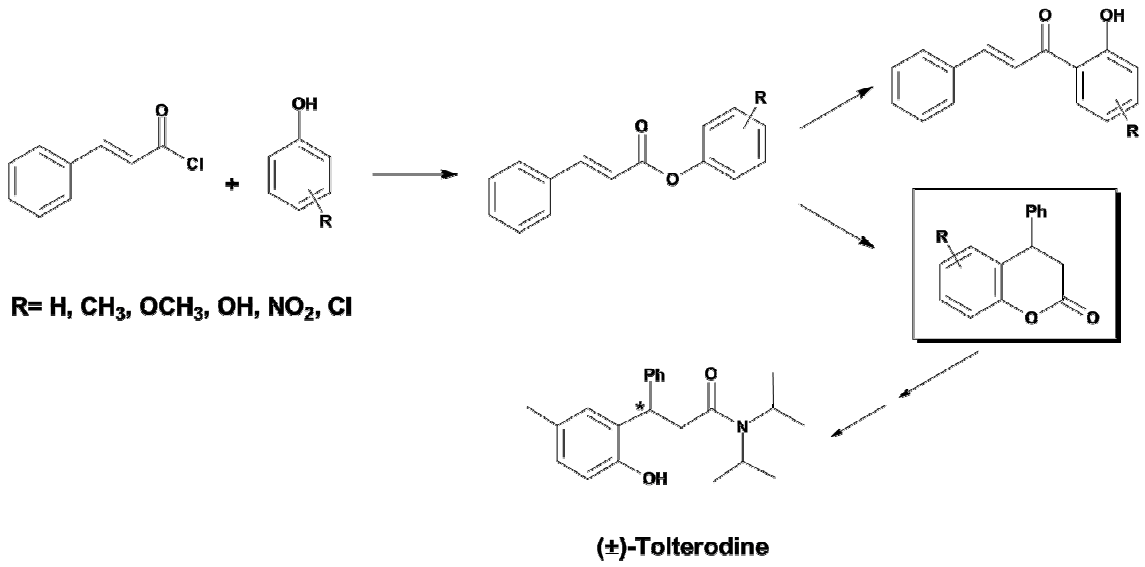
Synthetic Studies of Dihydrocoumarin and Chalcone Derivatives from Various Aryl Cinnamates : Devising a New Way to the (±)-Tolterodine

양덕모, *전제호, 전종갑

*한림대 화학과 *한림대 천연의약연구소*

Chalcones show antibacterial, antifungal, antitumor and anti-inflammatory properties. Some chalcones demonstrated the ability to block voltage-dependent potassium channels. They are intermediates in the biosynthesis of flavonoids, which are substances widespread in plants and with an array of biological activities. Many synthetic methods for 4-aryl-3,4-dihydrocoumarins have been reported up to the present, but most of the procedures based on the condensation of phenols with cinnamic acids in strong acidic media and at high temperature. In this study, dihydrocoumarin and chalcone derivatives were prepared by intramolecular cyclization and Fries rearrangement, respectively. The 4-pheny substituted 3, 4-dihydrocoumarin was transformed to racemic tolterodine, which is well known as a drug for cure of urinary urge incontinence and other overactive bladder (OAB) disorders.



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Microwave-assisted demethylation of methyl aryl ethers using ionic liquid

박지연, 박세경, 채정현

성신여대 화학과

A highly practical method for demethylation of methyl aryl ethers using ionic liquid has been developed. In this reaction, methyl group of methyl aryl ethers was readily cleaved by nucleophile from ionic liquid under microwave irradiation. A variety of methyl aryl ethers were converted to the corresponding phenolic compounds in a good to excellent yield.

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Synthesis of Benzophenone-benzoate Derivatives and their Anti-inflammatory Effects

권은미, 전종갑

한림대 화학과

Benzophenone-benzoate 구조의 화합물들은 prostaglandin H synthase 에 의해 나타나는 arachidonic acid 로 인한 염증을 억제하는 작용이 있다고 알려져 있다. Prostaglandin 은 염증을 자극하고 지방조직에서 지방분해를 방지한다고 알려져 있다. 다양한 구조의 benzophenone-benzoate 화합물들을 DCC coupling, Fries rearrangement, S_N2 반응 등을 이용한 총 3 단계 반응을 이용하여 합성하였고, 합성한 화합물들을 MTT assay 와 Cresyl violet stain 염색법을 이용하여 항염증 효과를 측정하였다

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Organocatalytic enantioselective indium-mediated allylation N-benzoyl hydrazones

김성준, 장두옥

연세대 화학과

A facile and highly enantioselective indium-mediated allylation of N-benzoyl hydrazones using cinchona alkaloid derivatives is descibed. We have developed an enantioselective indium-mediated allylation of N-benzoyl hydrazones for the preparation of enantioenriched homoallylic amines in the presence of chiral salts. The reactions of allyl halides to various N-benzoyl hydrazones of aldehydes were performed, affording the addition adducts in high chemical yields with high enantioselectivity.

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Rhodamine-Based Fluorescent Probes for the Detection of Gold(III) Ions

이지현, 태진성

연세대 화학과

Gold has been used as a great source in human life from the health care of medical science and to the technology of electronics, nanoparticles and other industries. In the part of chemistry, gold is quite popular in the field of gold nano particle technology. Application of gold nano particle is widely used in DNA, drug, and biosensing of biological systems. Even though gold acts its role in biomatrial field, it has a sort of toxicity in itself. When gold is presented as a metal (Au0), it is least reactive, but when it is attacked by acids or slowly oxidized by H2O2 in biological systems, it turns out to be Au+ or Au3+. Among gold ions, gold(III) is known as highly toxic in biological system which binds to DNA and nervous system that can cleave proteins and harass them working regularly in body.So to detect gold(III) in biological system, we have developed two fluorescent probes for fluorogenic detection method. There hasn`t been so many cases of detecting gold(III) ion, using fluorescent probes. This way of method can provide simpler and high efficiency detection method of visually-recognizable. And it also can detect only gold(III) ion in nano-scaled circumstances and make it possible working in aqueous media.

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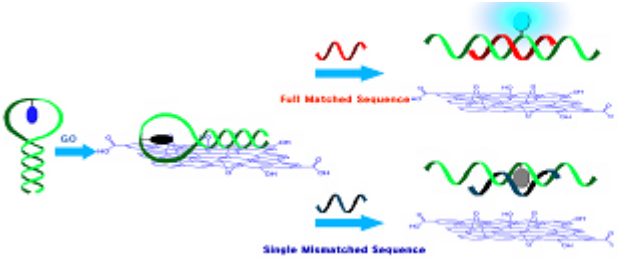
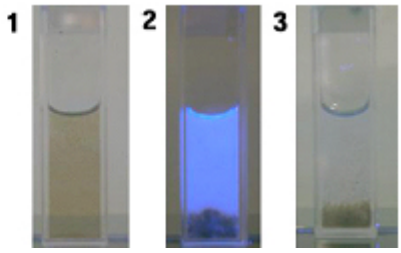
Graphene Oxide Enhances the Signal-to-Background Ratio of a Quencher-Free Molecular Beacon

이정우, 이일준, 김광수, 김병현

포항공과대 화학과

Since their invention by Tyagi and Kramer in 1996, molecular beacons (MBs) have been used widely for the detection of nucleic acids in genetic assays and biosensing devices, for the detection of single-nucleotide polymorphisms (SNPs), and in techniques based upon the polymerase chain reaction.1 The further development of MBs will require enhancements in their detection ability, namely their selectivity and signal-to-background (S/B) ratio. Previously, we reported2 a “quencher-free” (QF) MB that exhibits several advantageous features, including a high level of discrimination between the target and its single-mismatched congeners and economical device formation because of the absence of the quencher. Nevertheless, because of its intrinsic fluorescence, our quencher-free molecular beacon(QF-MB) exhibited a low S/B ratio of ca. 50%. Herein, we present GO greatly enhances the S/B ratios of QF-MB by reducing the background signal, particularly our QF-MB/GO system exhibited a higher S/B ratio (31.0) relative to that (2.2) of the same system in the absence of GO.





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Molecular recognition of dicarboxylic acid and cation through fluorescence excimer formation by cholesterol based imidazolium receptor

Md. Wasi Ahmad, Jadav Jyoti, 김홍석

경북대 응용화학과

A novel cholesterol-based fluorescent chemosensor has been designed and synthesized, where the imidazole are used as the binding site and the pyrene as the fluorophores. Dicarboxylic acids and cations are the most attractive targets for molecular recognition. Receptor shows enhanced excimer emission fluorescence in EtOH toward malonic acid and Hg^{2+} ions.

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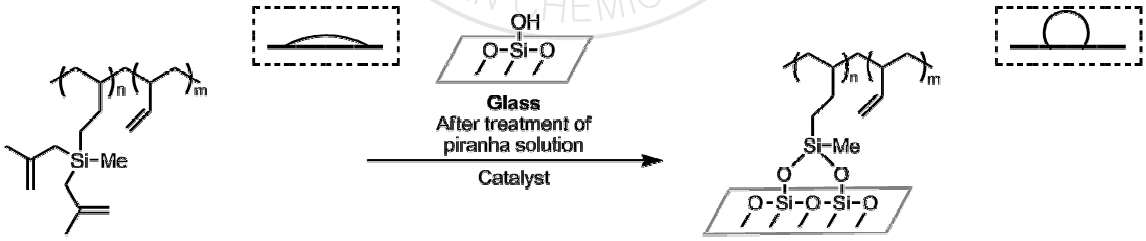
Catalytic Immobilization of Derivatives Polybutadiene onto Solid Support

최지환, 전철호

연세대 화학과

Fabrication of high performance organic-inorganic hybrid has been still attracted attention in organic and material chemistry. Recently, we found highly efficient catalytic immobilization method using stable organoalkenylsilanes. With this protocol, we have developed a novel immobilization method of organic molecules using polybutadiene as a mediator, which has many vinyl groups to be modified. For this purpose, methallylsilane-impregnated polybutadiene was prepared by hydrosilation of silane and polybutadiene, and then subsequent immobilization of silane-impregnated polybutadiene onto glass surface was carried out under acid catalyst.



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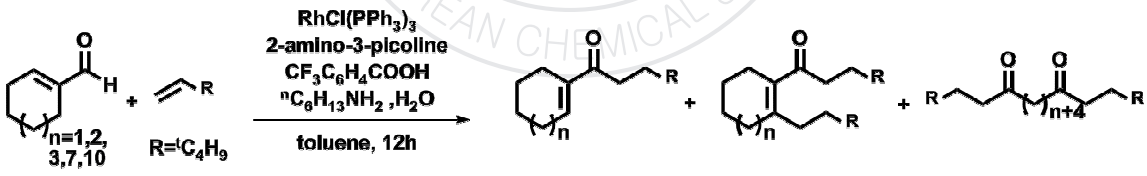
Synthesis of Diketone from Cycloalkene-1-carboxaldehyde through Hydroacylation and retro-Mannich type Reaction

이유라, 전철호

연세대 화학과

Transition-metal catalyzed C-H and C-C bond activation have been widely investigated for the synthesis of useful organic molecules. We have developed novel synthetic method for preparing diketones in one-pot from cycloalkene-1-carbaldehyde and 1-alkene. In this reaction, cycloalkene-1-carbaldehyde was converted to symmetric diketones by consecutive Rh(I)-catalyzed chelation-assisted hydroacylation and amine-mediated retro-mannich type fragmentation. The size of cycloalkene was important for generating diketones. We also applied this protocol to prepare asymmetric diketones using chiral myrtenal.



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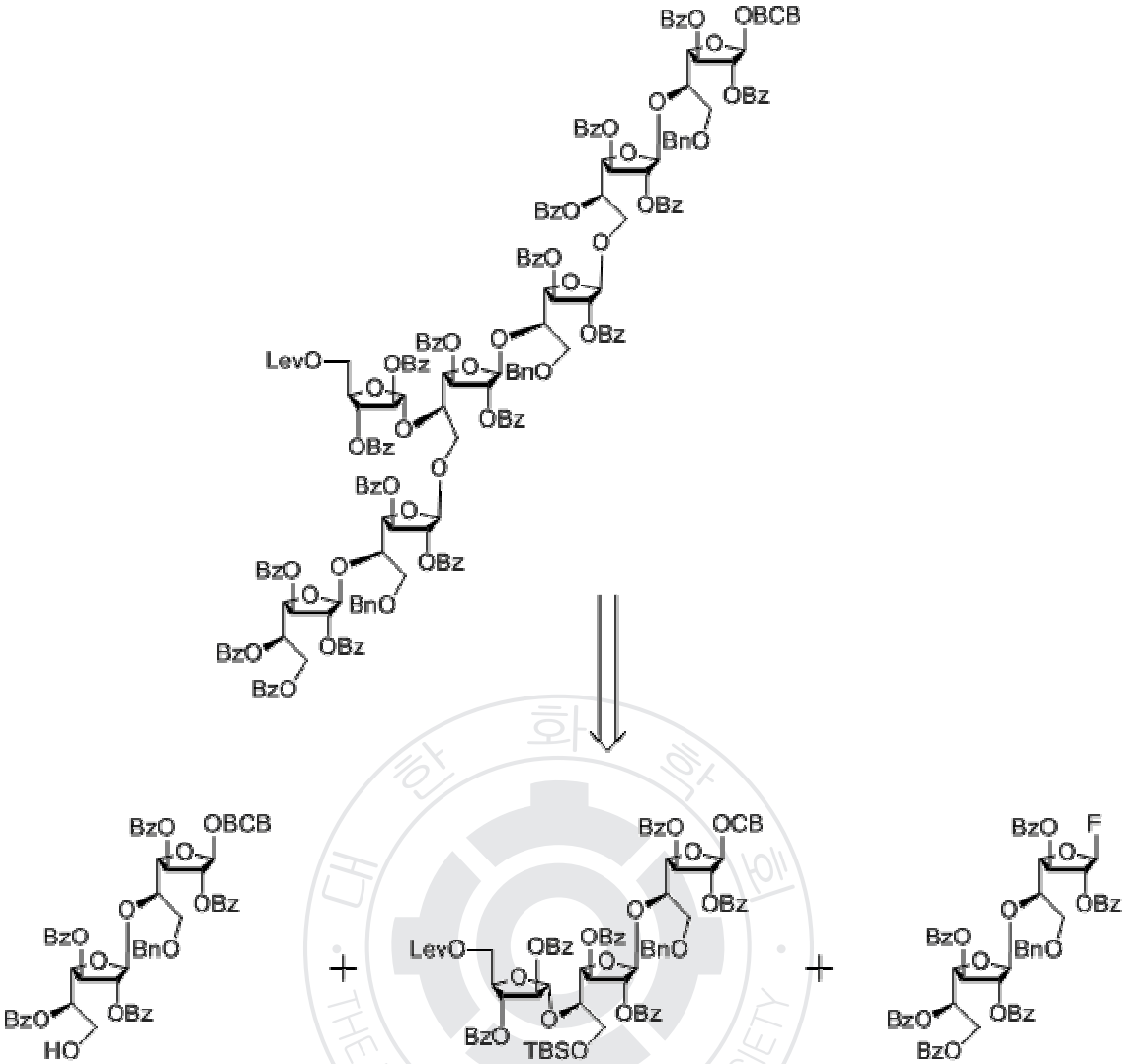
Stereoselective Synthesis of Heptafuranoside Subunit of Arabinogalactan from the Cell Wall of *Mycobacterium tuberculosis*

박정준, *김관수

*연세대 화학 *연세대 화학과*

The mycolyl arabinogalactan-peptidoglycan (mAGP) complex is known to be essential for the survival and pathogenicity of *Mycobacterium tuberculosis.* The synthesis of the mAGP motifs is important, owing to not only their potential as antitubercular drug, but also their biological significance as substrates for enzymes involved in the biosynthesis of mycobacterial cell wall. In this work, the synthesis of {β-D-Galf-(1→5)-β-D-Galf-(1→6)-[α-D-Araf-(1→5)]-β-D-Galf-(1→5)-β-D-Galf-(1→6)-β-D-Galf-(1→5)-β-D-Galf}, a suitably protected form of the heptafuranoside subunit from the arabinogalactan of Mycobacterium tuberculosis has been achieved by the preparation of seven monosaccharide building blocks with complete stereoselectivity, followed by the glycosylations using the prepared 2′-carboxybenzyl glycosyl and fluoroglycosyl donors.



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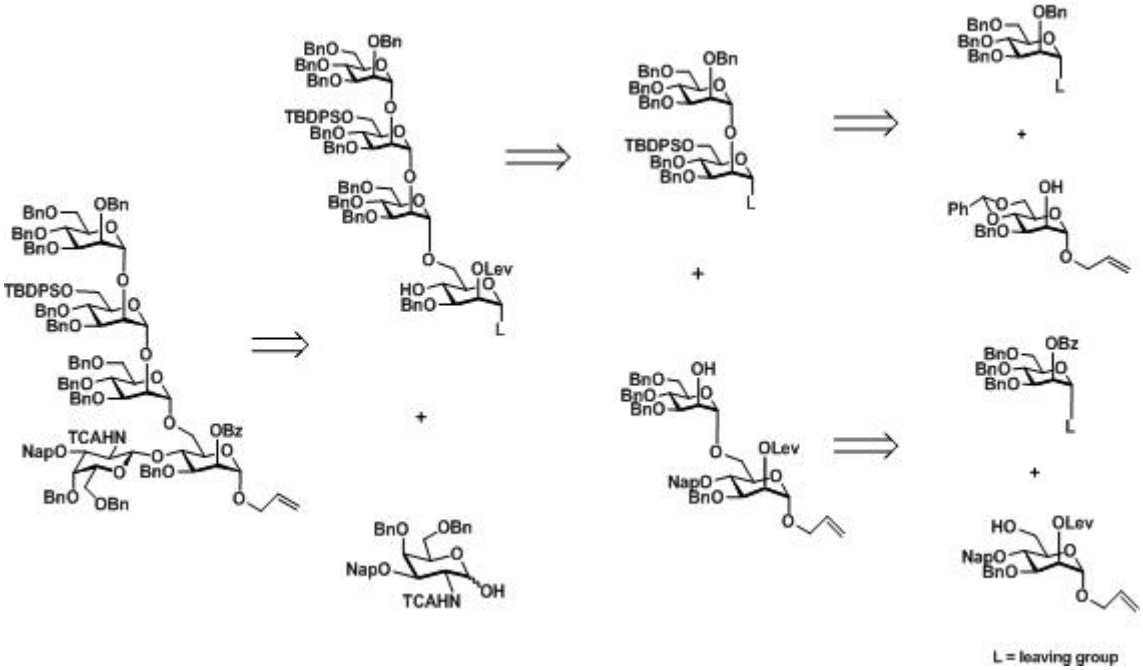
Synthesis of Pentasaccharide Subunit from Glycosyl Phosphatidyl Inositol Anchor of *Scrapie* Prion Protein

지예진, 김관수

연세대 화학과

The mad cow disease, bovine spongiform encephalopathy, is a fatal, neurodegenerative disease in cattle, which generates spongy in the brain and spinal cord. Many scientists think the disease as transmittable to human beings by taking the brain and spinal cord of infected cattle. In an effort to study important biological functions of the mad cow disease and to develop the chemotherapy agents, it is essential to synthesize the glycosyl phosphatidyl inositol (GPI) anchor, which connects *Scrapie* prion protein via their *C*-terminus to eukaryotic cell membranes. In the present work, the synthesis of {α-D-Manp-(1→2)-α-D-Manp-(1→2)-α-D-Manp-(1→6)-[β-D-GalNAcp-(1→4)]-α-D-Manp}, a suitably protected form of pentasaccharide unit of GPI anchor of *Scrapie* prion protein was achieved by the preparation of five monosaccharide building blocks with careful stereo- and position-manipulations, and then by stereoselective glycosylations of trichloroacetimidate donors in the stereoselective manner.



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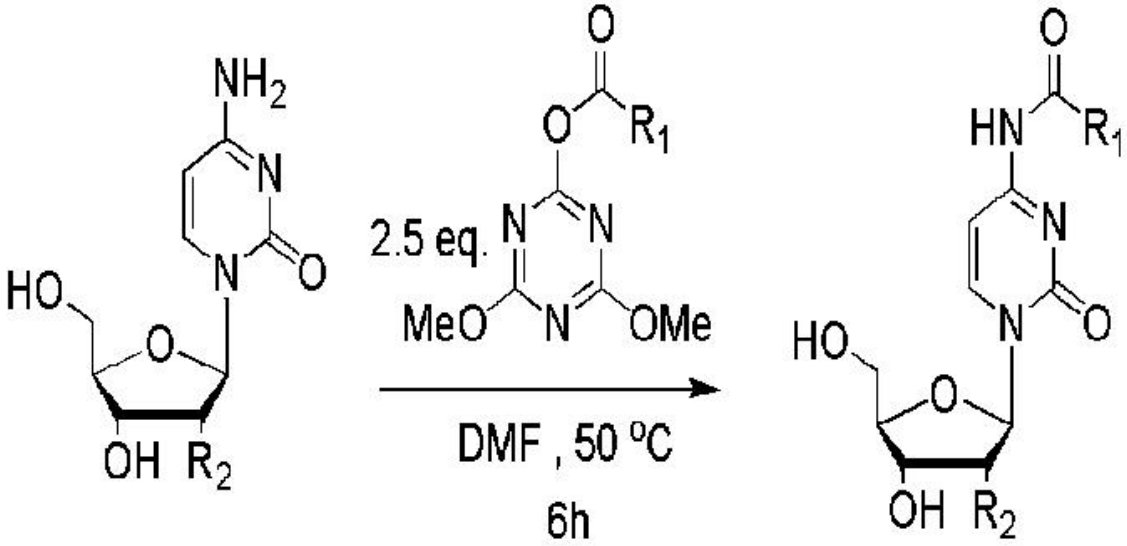
An efficient one-pot N-acylation of deoxy- and ribo-cytidine using carboxylic acids activated in situ with 2-chloro-4,6-dimethoxy-1,3,5-triazine

Ambadas B. Rode, 홍인석

공주대 화학과

The use of carboxylic acids with 2-chloro-4,6-dimethoxy-1,3,5-triazine (CDMT) for the selective preparation of N4-acetyl, benzoyl and phenoxy acetyl derivatives of cytidine and 2′-deoxycytidine is reported. The strategy presented here eliminates the need for the temporary masking of the hydroxyl groups of nucleosides required in conventional procedures. This novel cost-effective single-step protection strategy is advantageous in bulk production and was found to readily protect the exocyclic amine preferentially over the exposed alcohol functionalities. A similar approach was attempted for the protection of 2′-deoxyadenosine and 2′-deoxyguanosine, but was found to be unsuitable.



R_2= H , OH.

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Synthesis and Characterization of New fused heteroacene for OTFTs

정희정, 박지희, 천은정, 안진영, *권순기, 이상경

*경상대 화학과 *경상대 나노신소재공학부*

Organic semiconductors show great promise in various low-cost, large-area, electronic applications. Fused ring coplanar acenes, such as pentacene, have been shown to yield high-performance field-effect transistor(FET), qualifying them as active materials in p-type organic electronic devices. Fused heteroacenes are good for semiconductor because of their excellent electronic properties, stability under ambient conditions, and ease of chemical modification. Fused heteroacenes have high charge-carrier mobility and excellent optical properties.Therefore we want to prepare and test for electronic properties of a new fused heteroacene , the results reported in this poster.

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Environmentally Friendly Method for Synthesis of Benzo[d]thiazoles

천은정, 박지희, 정희정, 안진영, 이상경

경상대 화학과

Organic reactions in aqueous media have increasingly attracted the attention of synthetic chemists, because water is one of the most abundant, cheapest, non toxic and environmentally friendly solvent. Keeping in our mind this theme of green chemistry, we examined the potential for using alternative benign reaction media for the synthesis of benzo[d]thiazole derivatives. Substituted derivatives of benzo[d]thiazole show several interesting biological properties, for instance antimicrobial or antimycobacterial, and are also used in the preparation of dyes and organic synthesis of the thermostable polymers and herbicides acting as photosynthesis inhibitors.We want to prepare benzo[d]thiazoles under environmentally friendly conditions. The results are followings the reactions of 2-aminobenzenethiol with acetyl chloride, 4-methoxybenzoyl chloride, 2-thiopheneacetyl chloride, etc in ordinary water and neat in the absence of any acid/base catalyst afforded the heterocyclic benzo[d]thiazole derivatives in good yields.

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Synthesis and Characterization of Anthracene Derivatives for OTFTs

박지희, 정희정, 천은정, 안진영, *권순기, 이상경

*경상대 화학과 *경상대 나노신소재공학부*

Recently, organic semiconducting molecules were very attractive for the fabrication of organic thin film transistors (OTFT) in various molecular electronics applications, such as flexible display, smart card, RF tag, and electronic paper. 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 $cm^2/(V s)$ 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. Since, we wanted to improve the charge carrier mobility. So, we designed a series of asymmetric anthracene derivatives, and synthesized for studies of characterization.

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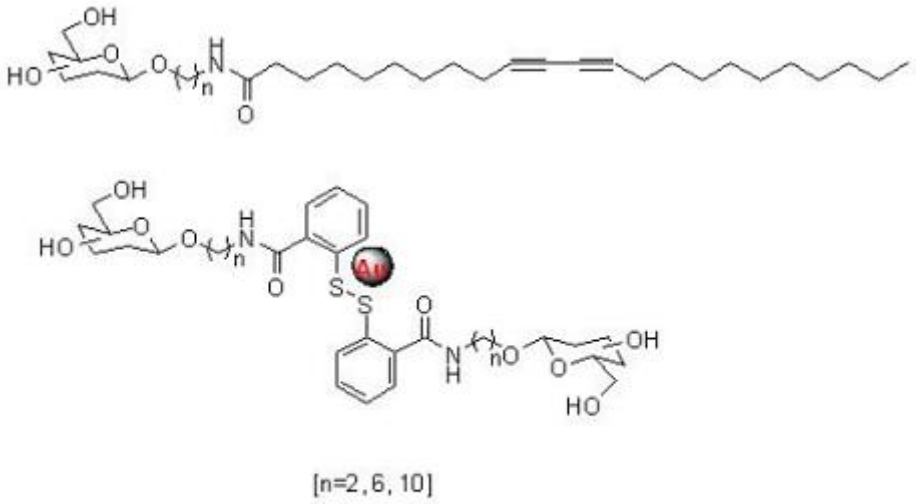
Luminescent Functionalization of Anomeric Center in Carbohydrate Derivatives: Application to Bio-Sensor Technologies

장은희

창원대 화학과

The luminescent functionalization of carbohydrates as a biosensor is important to recognize the specific cell surface. In this paper, 1) we will present the prepartation of PCDA and gold nanoparticle functionalization of anomeric center in glucose and galactose. 2) The connecting method between carbohydrate and functional group(PCDA and GNP) with a different carbon tether(n=2, 6, 10) will be presented too.



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Synthesis and Characterization of New Iridium Complex for OLEDs

안진영, 박지희, 정희정, 천은정, 김윤희, 이상경

경상대 화학과

Advances in organic light-emitting diodes (OLEDs) have triggered intensive research effort towards the development of efficient phosphorescent materials owing to their excellent performance and potential applications in OLEDs for full-color flat-panel display technology and light-emitting electrochemical cells (LECs).OLED screens have a number of advantages over conventional liquid crystal display (LCD) screens. Most importantly, light produced by OLEDs comes directly from the organic polymers that make up the display, rather than shining through coloured filters as in LCD screens. The device efficiency and emission color of iridium-based OLEDs can be modified easily by tuning the structure of the organic-ligand chromophore. The best materials for this purpose are complexes of iridium(III) with large cyclic ligands that good stability, a rapid response time, and access to colours across the visible spectrum. So, we decided to prapare new iridium complex by reaction $Ir(acac)_3$ with 2-(biphenyl-3-yl)pyridine. The desired iridium complex obtained with moderate yield and checked the physical properties.In this poster, we report the synthetic route and physical properties of new iridium complex.

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Synthesis, Characterization, and Physical Properties of CyclometalatedIridium(III) Complexes

강현희, 오대환, 소기호, *권순기, 김윤희

*경상대 화학과 *경상대 나노신소재공학부*

Currently, organic electroluminescent (EL) devices are an active area of research because of their potential applications in flat-panel displays. The research to synthesize phosphorescent materials with heavy metals such as platinum and iridium has attracted considerable attention because an internal quantum efficiency of 100% can be achieved by the energy transfer from both the singlet and layer.In this research, we designed and synthesized new iridium complex. And the physical properties of new iridium complex will be discussed.

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Enantioselective Iridium-Catalyzed Carbonyl Allylation from the Alcohol or Aldehyde Oxidation Level via Transfer Hydrogenation

김인수

울산대 화학과

Carbonyl allylation is a core synthetic method and gateway to polyketide natural products. Despite enormous effort, the vast majority of carbonyl allylation protocols rely upon the use of preformed allyl metal reagents. Pursuant to the first carbonyl allylations mediated by isolable allylboranes (1964) and allylsilanes (1976), enantioselective carbonyl allylations employing chirally modified allyl metal reagents were established, as first reported by Hoffmann (1978). A potentially more attractive approach to carbonyl allylation involves the use of allylic acetates, alcohols and halides as allyl donors. This approach requires reductive generation of allyl metal species and, to date, stoichiometric metal-based terminal reductants are required for catalytic turnover. Herein we describe how the union of carbonyl addition and hydrogenation chemistry has evoked a new suite of catalytic methods for enantioselective carbonyl allylation. Unlike classical methods for carbonyl allylation, the hydrogen-mediated variants occur in the absence of stoichiometric allylmetal reagents, minimizing or entirely excluding generation of stoichiometric byproducts. Additionally, under transfer hydrogenation conditions, alcohols may serve dually as hydrogen donors and aldehyde precursors, enabling carbonyl addition directly from the alcohol oxidation level, thus circumventing redox manipulations required for discrete generation of carbonyl electrophiles. These protocols are among the first methods available for direct catalytic C-H functionalization of alcohols at the carbinol position.

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Enantioselective Iterative Two-Directional Carbonyl Allylation and Its Application to the Total Synthesis of (+)-Roxaticin

김인수

울산대 화학과

Nature's vast collection of polyketide natural products comprises thousands of compounds incorporating polyacetate-derived 1,3-diol or higher 1,3-polyol substructures. Although numerous procedures for the synthesis of these ubiquitous structural motifs have been advanced, the iterative allylmetallation of aldehydes has found exceptionally broad use. For example, asymmetric iterative allylchromation (Nozaki-Hiyama coupling), allyltitanation, allylstannation, allylsilation, and allylboration have been employed in synthetic approaches to 1,3-diols and higher homologues. Brown's allylborane has found the most extensive use in iterative asymmetric carbonyl allylation. Although super-stoichiometric generation of isopinocampheol poses a barrier to large-volume applications, both enantiomers of α-pinene are available at low cost and excellent levels of stereocontrol are observed, making the Brown method attractive for use in academic laboratories. However, use of traditional allylmetallation procedures in iterative two-directional syntheses of 1,3-polyol substructures is prohibited by the instability of malondialdehyde. The ability to perform carbonyl allylation from the alcohol oxidation level enables allylation process that cannot be performed from the aldehyde oxidation level. Under the conditions of C-C bond forming transfer hydrogenation, substituted 1,3-propanediol and higher 1,n-diols are subject to successive generation to provide C2-symmetric adducts in good yield with complete levels of catalyst-directed diastereoselectivity. To illustrate the utility of this approach, the polyene macrolide (+)-roxaticin was prepared in a total of 21 steps from 1,3-propane diol.

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Blue Light Emitting Material with Limb Structure

박현태, 강문성, 김윤희, *권순기, 이상경

*경상대 화학과 *경상대 나노신소재공학부*

Since the discovery of multilayered organic light emitting diodes (OLEDs) by Tang et al. electroluminescent devices have been the subject of intensive investigation because of their applications in full-color displays. For the full color display, three basic colors- red, green and blue- are needed. Particularly, in terms of efficiency and color purity for full color applications, the blue emitting devices have to be improved. Thus, recent various studies have been focused on improving the blue emitting material. In this research, we designed and synthesized new blue emitting material based on anthracene. anthracene derivatives have interesting photo and electroluminescent properties and good electrochemical properties. They have been extensively studied in applications such as light emitting diodes.

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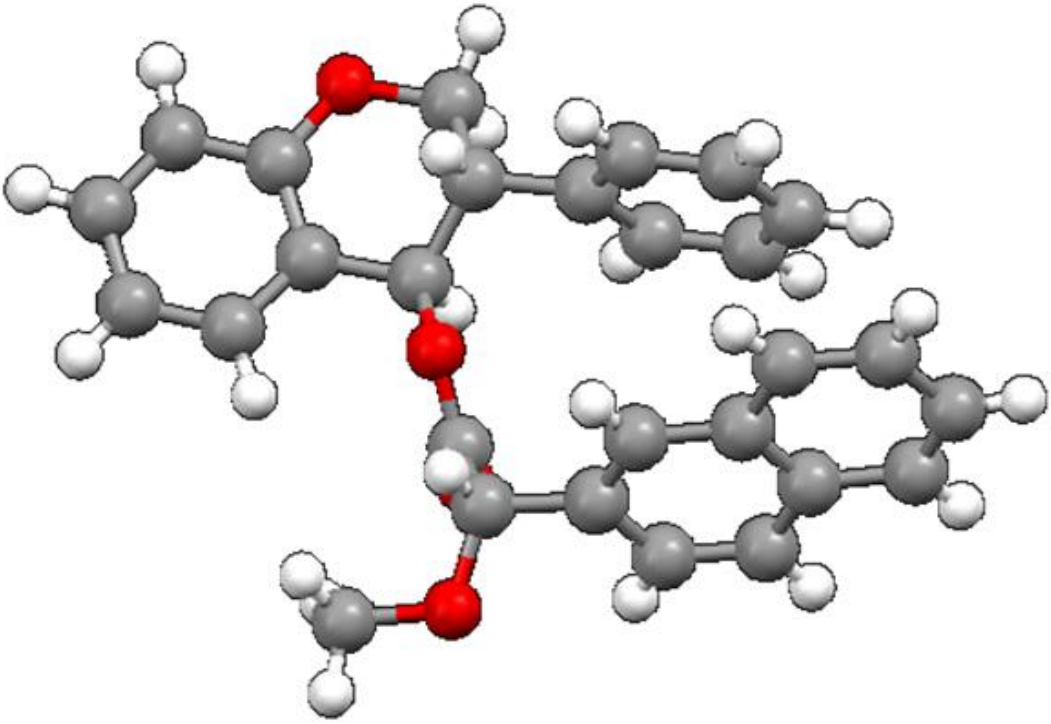
Absolute Structure Anlaysis of Isoflavanol Stereoisomers

원동호, 한재홍

중앙대 생명공학과

Due to the biological importance and especially related to the *S*-equol biosynthesis, *cis*- and *trans*-isoflavanol were synthesized from the reduction of isoflavone. Enantiomers of *cis*, and *trans*-isoflavanol were further isolated by Sumi-chiral column chromatography, and characterized by UV-VIS, IR, and NMR spectroscopy. Absolute configurations of stereoisomers were determined by computational chemistry-assisted CD (circular dichroism) spectroscopy, including ECD and VCD. In addition, each enantiomer of *cis*-isoflavanol and *trans*-isoflavanol was derivatized with *R*-2NMA (Naphthylmethoxyacetic acid) and *S*-2NMA, respectively, and their absolute configurations were determined by the modified Mosher method, utilizing the empirical chiral recognition by the anisotropic shielding effect of the chiral derivatizing group. Finally absolute configuration of the stereoisomers was confirmed by single crystal X-ray crystallography.



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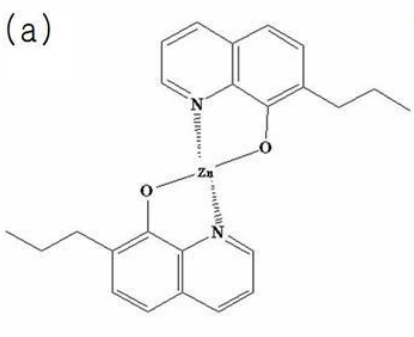
A Propylquinoline Zinc Complex : Synthesis and Electroluminescence Characteristics

김재성

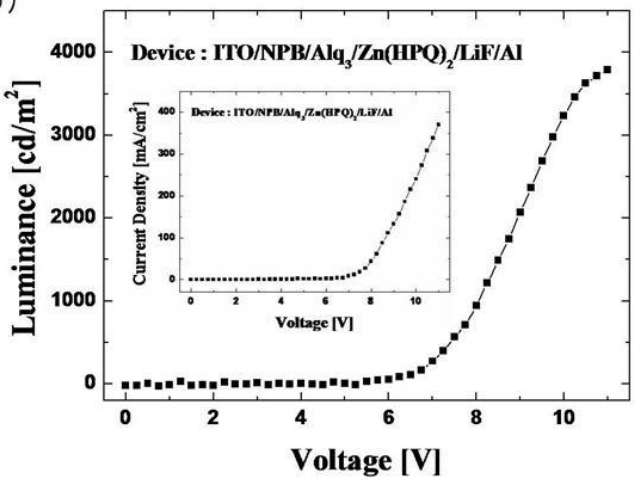
인제대 화학과

Jae-Sung Kim, Burm-Jong LeeDepartment of Chemistry & Institute of Functional Materials,Inje University, 621-749, Gimhae, KoreaE-mail : chemlbj@inje.ac.kr Metal-chelate materials based on polycyclic aromatic ligands are attractive for tuning emission colors. The metal-chelate materials emit various luminescence colors depending on the molecular structure. An emission material, bis(8-hydroxy-7-propylquinoline) zinc [$Zn(HPQ)_2$], was synthesized for organic light-emitting devices. The color of $Zn(HPQ)_2$ was yellow in a visible ray, but it changed to yellow-green in a ultraviolet ray. The structure of $Zn(HPQ)_2$ was determined by FT-IR, FT-NMR, UV-Vis and elemental analysis. The thermal stability was measured by TGA. The photoluminescence (PL) of $Zn(HPQ)_2$ was measured in the chloroform solution with maximum wavelength of 555 nm. The HOMO and LUMO energy levels of $Zn(HPQ)_2$ were estimated from the measurement of cyclic voltammetry. The devices with structure of ITO/NPB/$Zn(HPQ)_2$/Alq3/LiF/Al were constructed to investigate their electroluminescent (EL) performance. The EL shows the maximum wavelength at 520 nm and the turn on voltage of the device of 7V. The maximum luminance of the device shows approximate 4000 cd/m^2 when the voltage at 11V. Fig. (a) The chemical structure of $Zn(HPQ)_2$ and (b) I-V-L characteristics of the device using $Zn(HPQ)_2$ as emitting layer.

(a)



(b)



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Synthesis and Characterization of a New p-Type Organic Thin Film Transistors (OTFTs) Materials for Soluble Processed.

강문성, 박현태, 김윤희, *권순기

*경상대 화학과 *경상대 나노신소재공학부*

Conjugated oligomers and polymers represent one of the most important classes of advanced materials in recent years. The extensive amounts of research in the field are driven by the promise of low-cost processing applications that are typical of organic materials over their inorganic counterparts. The greatest advantage of organic materials is the diversity of structures and tunability of properties offered through molecular design. Recently, great studies have been made in areas such as thin-film transistors, light-emitting diodes, photovoltaic cells, and nonlinear optical devices. Thiophene-based materials have drawn considerable attention for their potential applications in the area of organic semiconductors because of their excellent chemical stability, high carrier mobility, and the ease of structural tuning to adjust the electronic, optical, and morphological properties. We synthesized new organic thin-film transistor material by Sonogashira reaction and Suzuki coupling reaction.

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Multi-Color Two-Photon Fluorophores for in Vivo Imaging

MASANTA GOUTAM, *김형중, **임창수, **조봉래, ***김환명

*아주대 분자과학기술연구센터 *아주대 에너지시스템학부 **고려대 화학과 ***아주대 에너지시스템학부, 분자과학기술연구센터*

TPM has the advantages of increased penetration depth (> 500 μm), localized excitation, and prolonged observation time. Using TPM, one can image intact tissue for a long period of time with minimum interference from tissue preparation artifacts that can extend more than 70 μm into the tissue slice.For maximum utilization of TPM, it is essential to develop efficient two-photon probes. However, most of the fluorescent probes presently used for TPM have small TP action cross sections (Φδ), demanding impractically high concentrations of probe and/or laser power. Herein, we describe a series of two-photon multi-color emissive dipolar molecules for various TP probes. These compounds can be easily synthesized, show appreciable water solubility, and emit strong two-photon fluorescence in the physiological condition.

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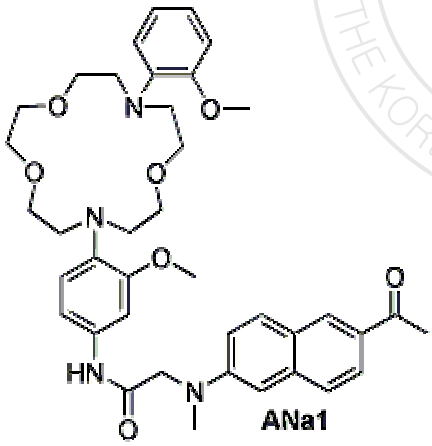
Sodium-Ion-Selective Two-Photon Fluorescent Probe for In Vivo Imaging

김미경, *임창수, 홍종태, *한지희, 장혜영, *조봉래, 김환명

*아주대 에너지시스템학부 *고려대 화학과*

We report a two-photon probe (ANa1) that shows strong two-photon excited fluorescence enhancement in response to Na^+, a dissociation constant (K_d^i) of 26 ± 2 mM in the cell, can be easily loaded into the cells, and can selectively detect $[Na^+]_i$ in live cells and living tissues at 100-200 μm depth for a long period time.



한국화학회 THE KOREAN CHEMICAL SOCIETY

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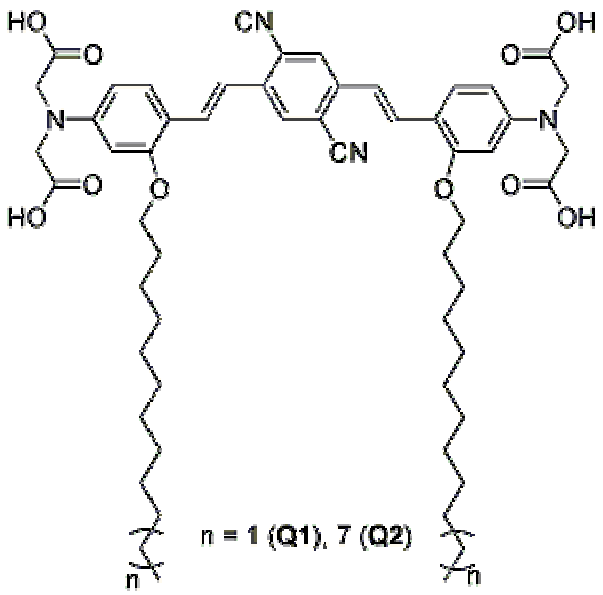
발표종류: 포스터, 발표일시: 목 10:30~12:30

Two-Photon Biomembrane Probes with Large Two-Photon Absorption Property

김미경, 백나영, *조봉래, 김환명

*아주대 에너지시스템학부 *고려대 화학과*

The lipid rafts hypothesis postulates that plasma membrane has liquid-ordered domain, enriched in sphingolipids, cholesterol, and specific proteins, and liquid-disordered domain, enriched in unsaturated glycerophospholipid. An ideal tool for such purpose is two-photon microscopy (TPM) that utilizes two near-infrared photons for excitation. For an optimal TPM, it is crucial to develop efficient two-photon (TP) probes for specific applications. Herein, we report TP probes (Q1 and Q2) that show large TP absorption properties in physiological conditions and can visualize the lateral heterogeneity in cell plasma membranes in the live cells and intact tissues using two-photon microscopy without internalization problem.



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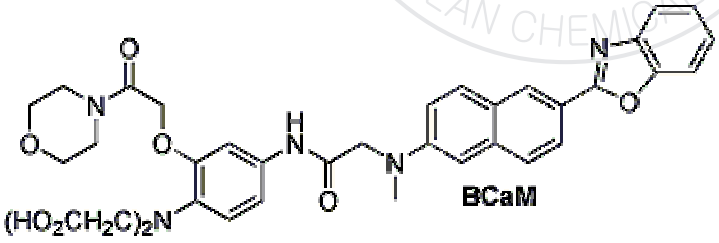
Visualization of Near-membrane Ca^{2+} in Living Tissue with a Two-Photon Probe

김형중, *한지희, *조봉래, 김환명

*아주대 에너지시스템학부 *고려대 화학과*

Calcium is a ubiquitous second messenger controlling numerous cellular functions. The near plasma membrane Ca^{2+} concentration ($[Ca^{2+}]_m$) is over the 10-fold higher than that of the bulk cytosolic Ca^{2+} and can reach > 100 μM upon activation. To investigate the changes in $[Ca^{2+}]_m$, we report a two-photon probe (BCaM) that meets all of the following requirements. 1) significant two-photon (TP) cross section for bright TP microscopy images, 2) small MW for cell loading, 3) low Ca^{2+} affinity and high selectivity for Ca^{2+} ions, 4) specific plasma membrane locations, and 5) high photostability.



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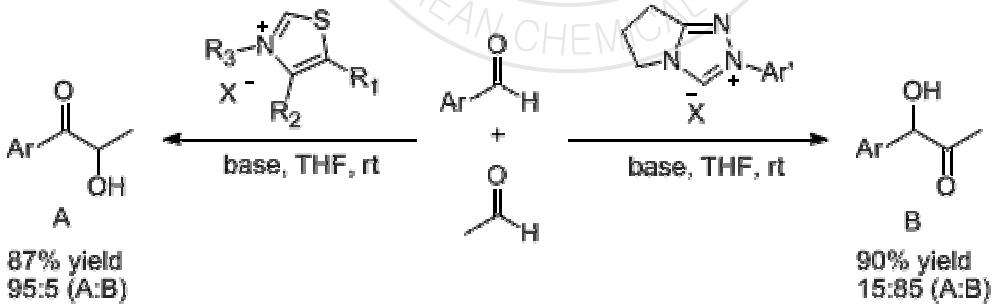
N-Heterocyclic Carbene-Catalyzed Highly Regioselective Intermolecular Cross-Acyloin Condensation of Acetaldehyde

JINMINGYU, 류도현, *양정운

*성균관대 화학과 *성균관대 에너지과학과*

Given the growing importance of acetaldehyde as simple nucleophile in organocatalytic reactions, we postulated that a practical and simple method for the preparation of acyl anion equivalent might be achieved if combined thiazolium and other azolium salt as carbene precursor with a base. We discovered that the generation of acyl anion equivalent from simple acetaldehyde, which successfully promotes the intermolecular cross-acyloin condensation of a variety of different aldehydes to give the corresponding acyloin condensation products in high yields with excellent levels of regioselectivity.



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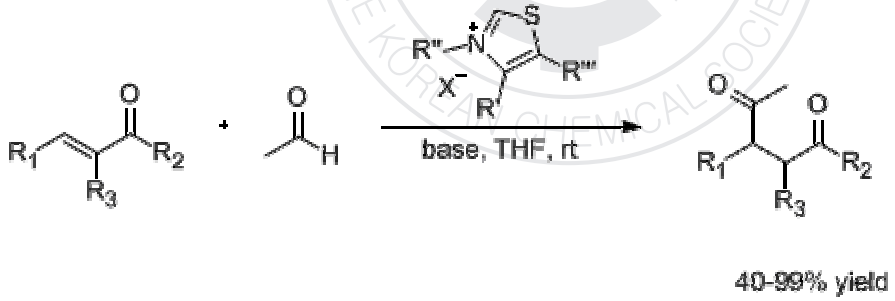
Intermolecular Stetter Reactions of Acetaldehyde using N-Heterocyclic Carbenes

JINMINGYU, 류도현, *양정운

*성균관대 화학과 *성균관대 에너지과학과*

The inversion of the normal mode of reactivity of aldehydes catalyzed by heteroazolium salt open up new synthetic pathways for the construction of carbon-carbon bonds. One appilication of this concept is an intermolecular Stetter reaction by using acetaldehyde as a simple nucleophile. We successfully discovered a new thiazolium salts catalyzed pathway for the synthesis of 1,4-dicarbonyl compounds.



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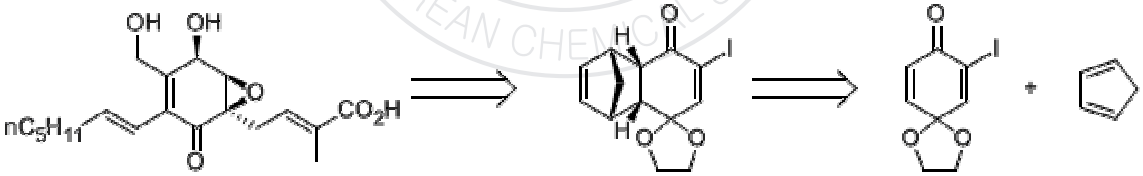
Synthetic studies on (+)-Ambuic acid

정선희, 서정원, 류도현

성균관대 화학과

Chiral cyclohexene epoxide compounds, frequently found in natural products, exhibit wide range of interesting biological active properties. Strobel and co-workers in a collaborative study in 2001, reported the isolation and structure determination of a novel, polyketide derived epoxyquinone natural product, (+)-ambuic acid From the culture extracts of Pestalotiopsis spp. And Monochaetia spp.A synthetic route to (+)-ambuic acid has been studied from the readily available chiral Diels-Alder adduct of cyclopentadiene and iodo-1,4-quinone monoketal. We expect that this novel synthetic route can be useful for the synthesis of various cyclohexene epoxide natural products.



Ambuic acid

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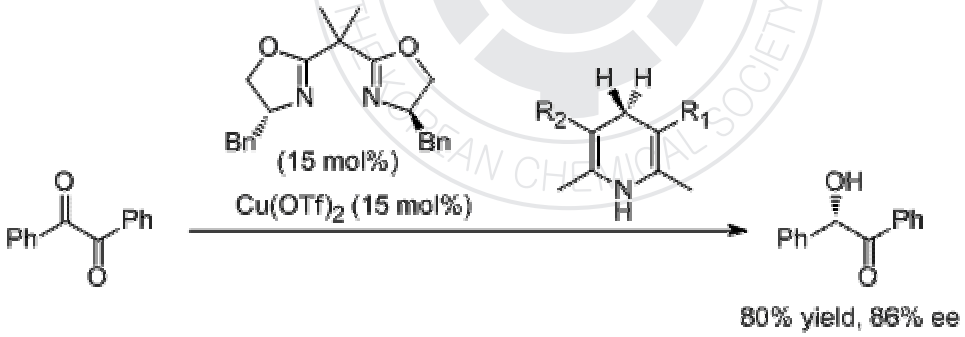
Catalytic Asymmetric Transfer Hydrogenation of α-Diketones with Hantzsch Esters

권영은, 류도현, *양정운

*성균관대 화학과 *성균관대 에너지과학과*

C2-symmetric chiral copper(II)-bisoxazolines function as alcohol dehydrogenase mimics and catalyze enantioselective transfer hydrogenations of α-diketones with Hantzsch esters as hydride source to give α-hydroxy ketones in good yields with excellent enantioselectivities.



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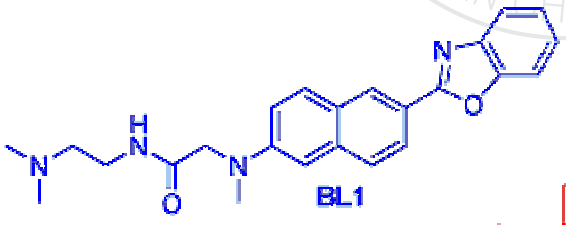
발표종류: 포스터, 발표일시: 목 10:30~12:30

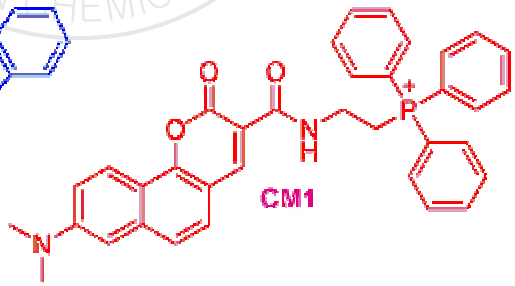
Two-Photon Dual-Color Trackers for Acidic Vesicles and Mitochondria in Vivo

박선근, 김미경, *한지희, *조봉래, 김환명

*아주대 에너지시스템학부 *고려대 화학과*

Two-photon microscopy has the advantages of increased penetration depth (> 500 μm), localized excitation, and prolonged observation time. Using TPM, one can image intact tissue for a long period of time with minimum interference from tissue preparation artifacts that can extend more than 70 μm into the tissue slice. To make it a versatile tool in biology, a variety of two photon probes for specific applications are needed. Herein, we report that BL1 and CM1 are capable of visualizing the acidic vesicles and mitochondria, respectively, and allow dual-color imaging these organelle in live cells and tissues at >100 μm depth for a long period of time.





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Solid Phase Asymmetric Alkylation Reactions Using 5,5-Dimethyl-2-phenylamino-2-oxazoline Chiral Auxiliary

N.P.B.Quynh, *김택현

*전남대 신화학소재공학과 *전남대 응용화학공학부*

Solid phase synthesis has emerged as a versatile and powerful technique in organic synthesis to prepare chemical libraries, because of its numerous advantages, such as its simple purification process as well as the easy recovery of the expensive reagents. However, stereoselective solid supported chiral auxiliaries still remain a relatively under-developed area. 5,5-Dimethyl-2-phenylamino-2-oxazoline chiral auxiliary has been reported to be a versatile auxiliary for asymmetric syntheses, exhibiting excellent levels of stereocontrol, greater stability and recyclability. In this study, we wish to report the preparation of a novel solid-supported chiral auxiliary based on 5,5-dimethyl-2-phenylamino-2-oxazoline and the preliminary results of our investigations concerning the asymmetric alkylation reactions on solid supports.

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Synthesis and Characterization of Host Material for Organic Light Emitting Diode Contaning Tetraphenylsilyl

오대환, 강현희, *김장주, **권순기, 김윤희

*경상대 화학과 *서울대 재료공학부 **경상대 나노신소재공학부*

OLED, getting the spotlight as a next generation display spends less eletric 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.In this research, we adopted tetraphenylsilane moiety for wide energy band gap(Eg), thermal-chemical stability, high efficiency and stability of a device. We synthesized and characterzed host materials for blue phosphorescence of OLED including tetraphenylsilane moiety.

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Investigation of Isothiouronium Salts Based on Anthracene and Pyrene: Isomerism and Anion sensing

정송이, *김택현

*전남대 신화학소재공학과 *전남대 응용화학공학부*

The design and synthesis of anion receptors have gained much attention in molecular recognition chemistry since anions play significant roles in biology. Recently, the ability of thioureas to complex anions has been thoroughly exploited in the field of molecular sensors due to the binding anions through hydrogen bonding. The use of isothiouronium groups has not been explored very much in the area of anion binding. Such groups would enhance the acidicity of the NH moieties and therefore can function as a better binder compared to the thiourea group. In this study, novel fluorescent anion chemosensors based on anthracene-bisisothiouronium and pyrene-isothiouronium were synthesized. These sensors contained two isomers in equilibrium and showed significant fluorescence enhancement upon the addition of fluoride, acetate and dihydrogen phosphate anions.

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Synthesis and Characterization of Novel Iridium Complexes Containing Trimethylsilyl Group for OLED Lighting

소기호, 강소희, 강현희, *권순기, 김윤희

*경상대 화학과 *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 achieve an efficient phosphorescent emitter.

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A Novel Synthesis of Ketones and *N*-Methoxy-*N*-methylamides from Pyrimidyl Diesters and Pyrimidyl Urethane Using Grignard Reagents

김민정, 박세빈, 이재인

덕성여대 화학과

4,6-Pyrimidyl diesters (1) and 6-methyl-2,4-pyrimidyl diesters (2) were newly prepared by the addition of 2 equiv of acid chlorides to a solution of 4,6-dihydroxypyrimidine and 2,4-dihydroxy-6-methylpyrimidine, respectively, in CH_2Cl_2 in the presence of 2 equiv of Et_3N at room temperature. The treatment of 1 and 2 with 2 equiv of Grignard reagents in THF afforded 2 equiv of ketones in high yields. 4,6-Pyrimidyl *N*-methoxy-*N*-methylurethane (3) was newly prepared by the addition of 2 equiv of *N*-methoxy-*N*-methylcarbamoyl chloride to a solution of 4,6-dihydroxypyrimidine in CH_2Cl_2 in the presence of 2 equiv of Et_3N at room temperature. The treatment of 3 with 2 equiv of Grignard reagents in THF afforded 2 equiv of *N*-methoxy-*N*-methylamides in high yields.

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Platinum catalyzed Hydrogenative cyclization of allene-aldehyde

홍종태, 장혜영

아주대 에너지시스템학부

The reductive cyclization of the allene and aldehyde is a very valuable method for forming a structure with the concomitant installation of two stereocenters. In an effort to expand the scope of platinum catalyst for the reductive coupling reaction, the Pt catalyst was applied to the hydrogen-mediated cyclization of the allene-aldehyde. Pt-complex generated from $PtCl_2$, and phosphine ligand, catalyzed the cyclization of allene-aldehyde under hydrogenation conditions to provide the desires product in reasonable yield. For the optimization of the reaction conditions, several phosphine ligands and additives were employed. In addition, control experiments were carried out to identify the catalytic reaction mechanism.

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발표종류: 포스터, 발표일시: 금 10:30~12:30

Synthesis of organocarboranes as Potential BNCT Agent

임현화, 이채호, *강상욱, **이종대

*원광대 생명나노화학부 *고려대 소재화학과 **조선대 화학과*

Carboranes are stable, lipophilic structures which resemble benzene in term of reactivity and bulkiness. Therefore it is not surprising that carborane-based biomolecules which an aromatic group is replaced by the boron cage have been prepared. Since carboranes which linked a biomolecule contain ten boron atoms, they theoretically may help deliver much higher concentrations of 10B atoms in cancer cells for boron neutron capture therapy (BNCT). Carboranylbenzothiadiazolidines containing water-soluble functional groups have been synthesized and evaluated growth inhibition of various tumor cell lines and boron corporation into B-16 melanoma cell.

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Stereoselective construction of oxabicyclic systems by an internal S_N2' enolate alkylation/ring-closing metathesis (RCM) strategy

윤정인, *이종국

*고려대 화학과 *한국화학연구원 난치성질환치료제연구센터*

Oxabicyclic systems have been found in many natural products and used as a bio-isoster of corresponding carbocyclic ones in pharmaceutical industry. We report here a novel route to a trans-1-oxabicyclic skeleton utilizing an intramolecular S_N2'enolate alkylation and ring-closing metathesis (RCM) as key steps.

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발표코드: **Ⅲ37P131포**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 금 10:30~12:30

Fluorescent Probe for Carbonyl Compounds

박석안, *김해조

*경기대 화학과 *경기대 이과대학 화학과*

A imidazolidine-functionalized coumarin (1) was utilized as a chemodosimeter for carbonyl compounds. The chemodosimeter has shown a selective and sensitive response to butadione over other various aldehydes or ketones through the oxidation reaction of imidazolidine to imidazole. When butadione were added, the fluorescence intensities of 1 were enhanced c.a. 54 times so that millimolar concentrations of butadione were detectable by the naked eye.

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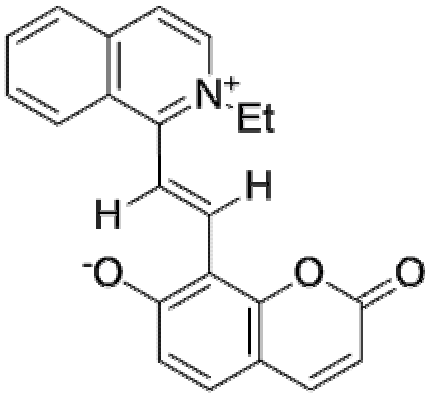
발표종류: 포스터, 발표일시: 금 10:30~12:30

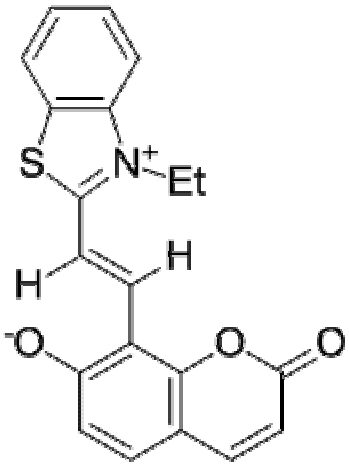
Negative Solvatochromism of Merocyanine Dyes: Their Application as a Probe for Water Contents in Organic Solvents

어수영, 차선영, 남궁지은, 장석규

중앙대 화학과

Two new merocyanine dyes were prepared and their signaling behaviors as a probe for water content in organic solvents were investigated. The coumarin based dyes exhibited a pronounced negative solvatochromism. Significant changes in absorption spectra in response to the changes in water content were conveniently analyzed by ratiometry. The solvatochromic behavior is particularly pronounced in lower water content region of less than 5% water. These dyes could be used as a chromogenic probe for the determination of water content in common water miscible organic solvents of acetonitrile, acetone, THF, and DMSO.





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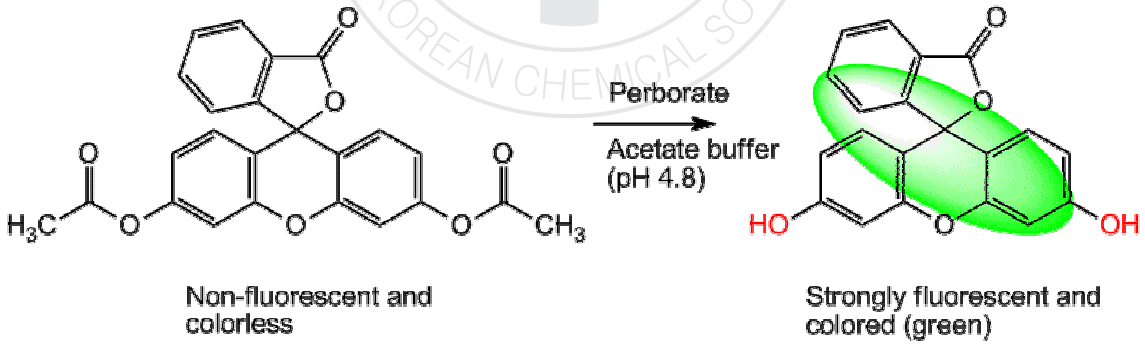
발표종류: 포스터, 발표일시: 금 10:30~12:30

Selective Perborate Signaling by Deprotection of Fluorescein and Resorufin Acetates

최명길, 박지은, 황지영, 장석규

중앙대 화학과

A new perborate-selective signaling system based on fluorescein was investigated. Diacetate derivative of fluorescein exhibited a prominent turn-on type response toward perborate ions in aqueous media. The signaling is based on the selective deprotection of acetate groups of probe by perborates, which resulted in significant chromogenic and fluorogenic signaling. Probe also exhibited a pronounced selectivity over other commonly used oxidants with a detection limit of 2.2 uM in a 90% aqueous acetonitrile solution.



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발표종류: 포스터, 발표일시: 금 10:30~12:30

Ratiometric Fluoride-selective Chemosignaling Behavior of Merocyanine Dye

차선영, 최명길, 김윤환, 장석규

중앙대 화학과

The fluoride-selective chemosignaling behavior of merocyanine dye was investigated. N-methylquinolinium based dye in the presence of phenylboronic acid showed fluoride-selective chromogenic signaling behaviors over other commonly coexisting anions in acetonitrile in micromolar concentration range. The signaling is due to the fluoride induced displacement of dye, which is associated with phenylboronic acid, that resulted in a significant chromogenic signaling of fluoride ions. The signaling is successfully analyzed by the ratiometric analysis of the absorption changes in response to the changes in fluoride ions. Phenylboronic acids having substituent of electron withdrawing group were found to exhibit more pronounced signaling behavior.

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발표종류: 포스터, 발표일시: 금 10:30~12:30

Enantioselective [3+2]-Dipolar Cycloaddition of Azomethine Ylide Generated from Nitrone-Alkyne Substrates via Gold Catalysis

정재원, 신승훈

한양대 화학과

8-Azabicyclo[3,2,1]octane forms the common core of wide range of biologically active natural products. Accordingly, efficient synthesis of this skeleton with high level of enantio-control has attracted considerable attention. Recently, our group has been developing nitrone or oxime-mediated redox reactions under the catalysis of Au-complexes. For example, the redox reaction between a nitrone and an alkyne generates azomethine ylide in-situ, in a completely atom-economical fashion which, in turn, participates in a subsequent tandem [3+2] dipolar cycloaddition. However, asymmetric version of this reaction remains unmet challenge yet. Considering the lack of precedents of asymmetric catalysis using Au(III)-complexes, we report here an auxiliary-based approach for the asymmetric [3+2] dipolar cycloaddition. For this purpose, we prepared enantiopure hydroxylamine derivatives and have shown that its nitrone derivatives underwent a smooth Au-catalyzed dipolar cycloaddition with tethered dipolarophiles in >99 % de, and therefore >99 % ee after deprotection of the auxiliary group.

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발표종류: 포스터, 발표일시: 금 10:30~12:30

Acid-catalyzed benzidine rearrangement of bis[4-(2-furyl-5-methyl)phenyl]diazane.

박희근, 정동훈, 박균하

충남대 화학과

Benzidine rearrangement refers to a reaction in which hydrazo (-NHNH-) group is broken, leading to the formation of the C-C or C-N bonds between two aryl groups. In this work, we report the unusual rearrangement of bis[3-(2-furyl)-4-methylphenyl]diazane prepared from corresponding azo compound. After benzidine rearrangement in aqueous ethanol solution, we were able to find that major pathway was the disproportionation (formation of azo and fission amine) accounting for about 70% conversion based on starting substrate. Besides this disproportionation products, we isolated a very small amount (about 10%) of rearrangement product in which one furyl ring is lost by [5,7]-sigmatropic shift. Currently extensive work is undergoing to clarify the unprecedented example of [5,7]-sigmatropic shift rearrangement.

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발표종류: 포스터, 발표일시: 금 10:30~12:30

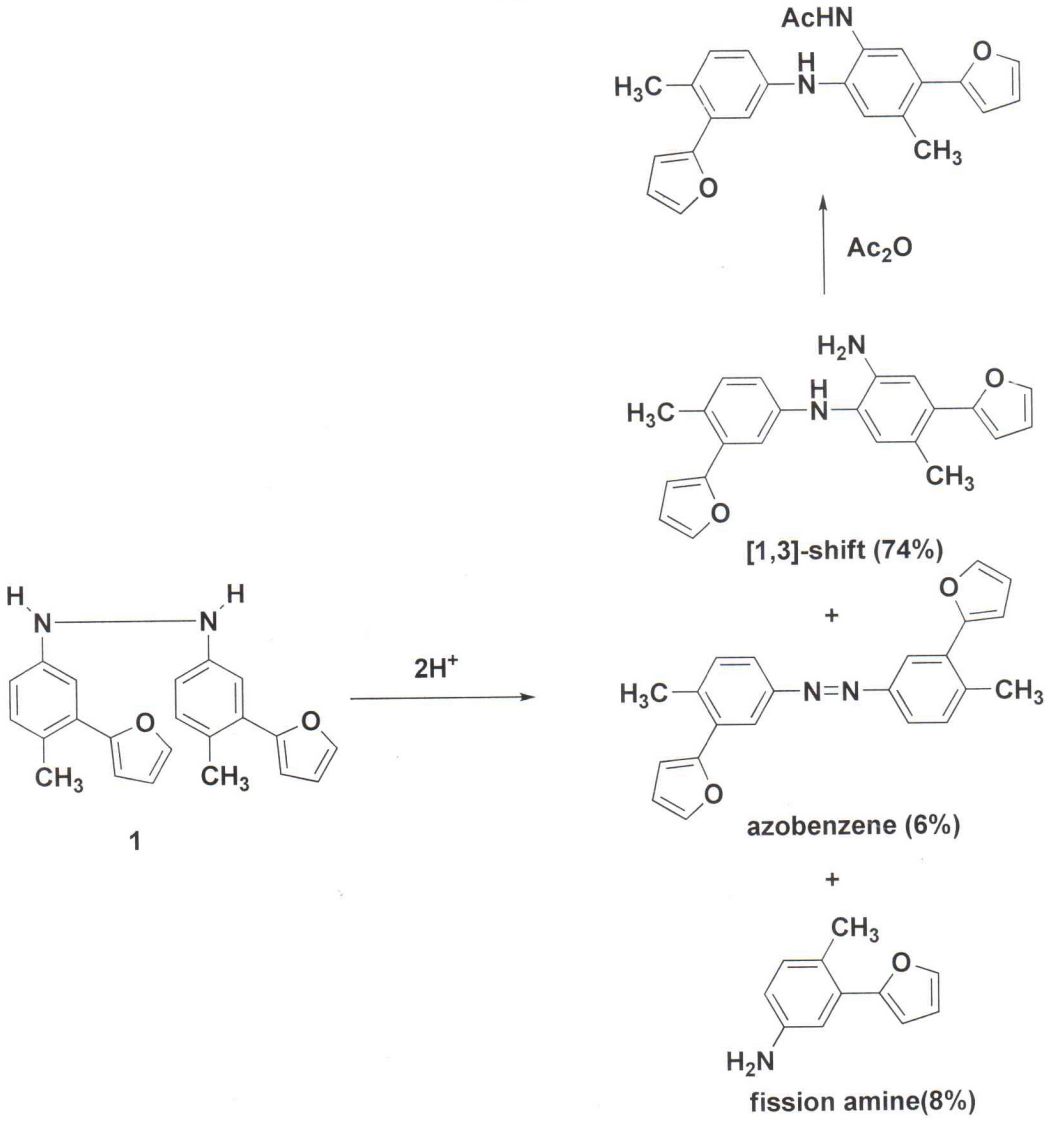
Acid-catalyzed benzidine rearrangement of bis[3-(2-furyl)-4-methylphenyl]diazane.An example of [1,3]-sigmatropic shift.

강명구, 정동훈, 김정권, 박윤봉, 허정석, 박균하

충남대 화학과

Bis[3-(2-furyl)-4-methylphenyl]diazane (1) was prepared from bis[3-(2-furyl)-4-methylphenyl]diazene was set to acid-catalyzed benzidine rearrangement in acidic ethanol solution. Product analysis showed that the rearrangement proceeded by [1,3]-sigmatropic shift together with disproportionation. The structures of products were determined by conventional spectroscopic data such as ^{1}H NMR, IR, elementary analysis and MALDI-MS. Acetylated product was used for ^{1}H NMR, elementary analysis and MS measurements. We were able to determine the ratio of products quantatively as [1,3]-sigmatropic shift product (74%) and disproportionation in 14%.

Scheme


AcHN
H
N
H3C
O
CH3
O
Ac2O
H2N
H
N
H3C
O
CH3
O
[1,3]-shift (74%)
+
O
H3C
N=N
CH3
O
azobenzene (6%)
+
CH3
O
H2N
fission amine(8%)
H
N
N
H
2H+
O
O
CH3
CH3
1

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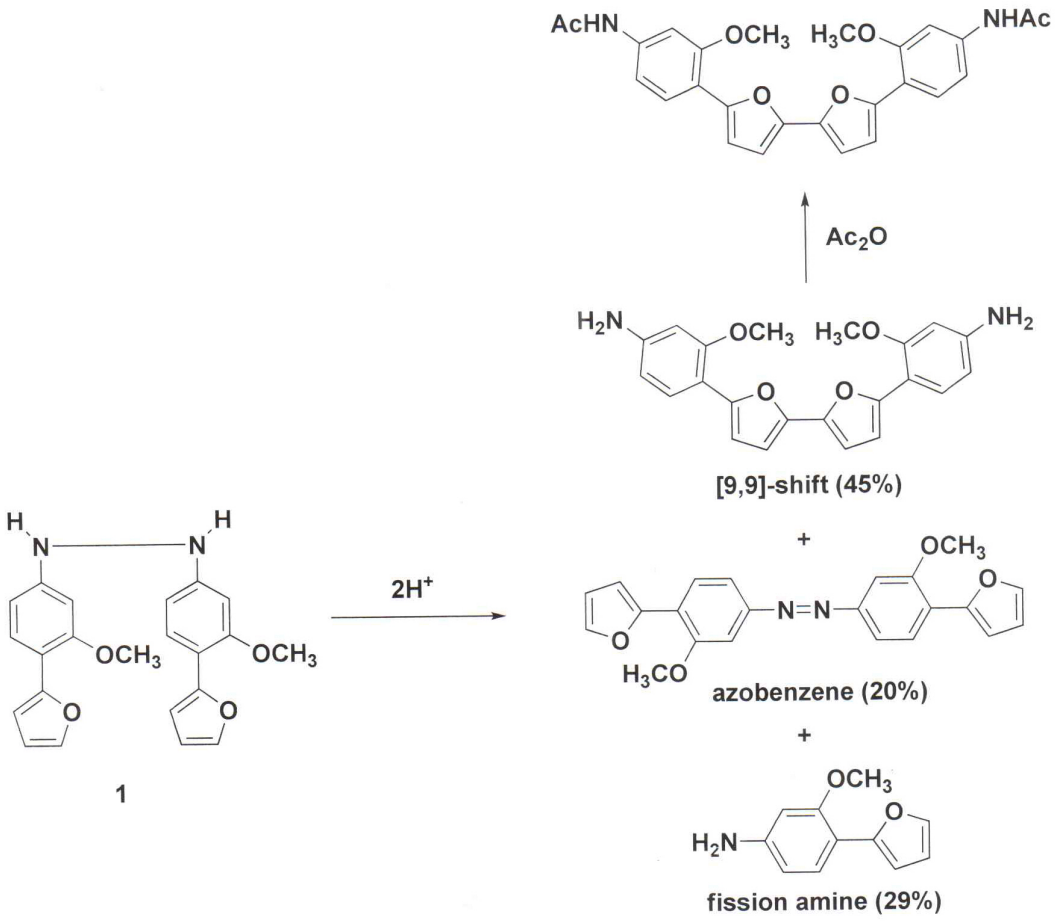
Acid-catalyzed benzidine rearrangement of bis[4-(2-furyl)-3-methoxyphenyl]diazane.An example of [9,9]-sigmatropic shift.

정동훈, 강성권, 박균하

충남대 화학과

Bis[4-(2-furyl)-3-methoxyphenyl]diazane (1) prepared by reduction of corresponding bis[4-(2-furyl)-3-methoxyphenyl]diazene in the conventional reaction conditions was subjected to acid-catalyzed benzidine rearrangement. After work-up, we isolated and determined the structure of the rearrangement product to p-benzidine type {[9,9]-sigmatropic shift (45%)}, based on ^{1}H NMR. Elementary analysis was performed with the use of the acetylated rearrangement product. Beside this rearrangement product, we found out that disproportionation also proceeded yielding azo and fission amine (49%) as shown in the scheme. This [9,9]-shift provides another example to our first report on [9,9]-shift.

Scheme



KOREAN CHEMICAL SOCIETY

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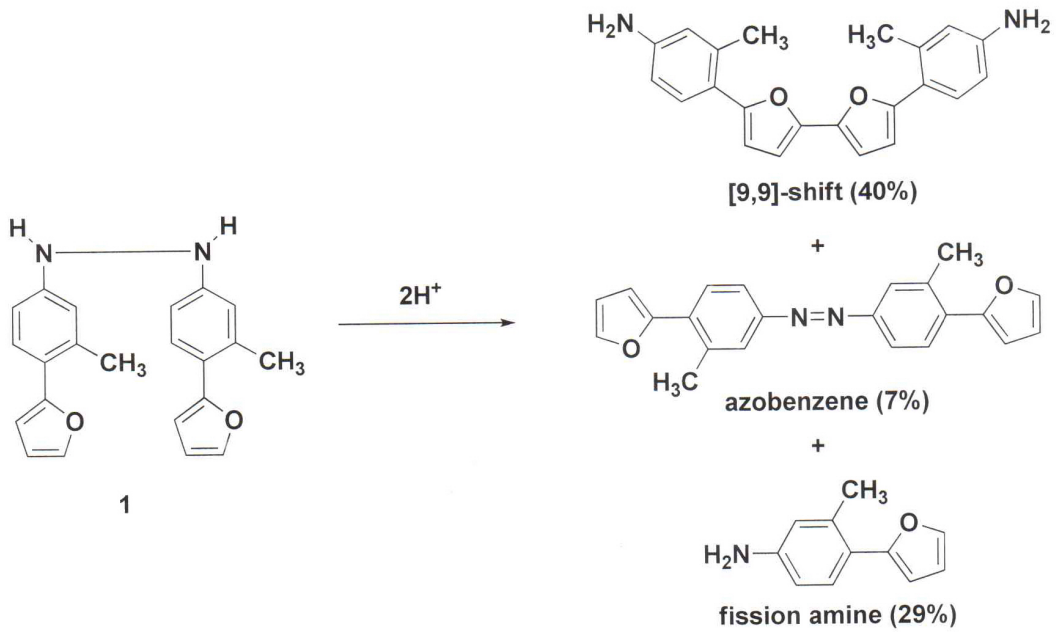
Acid-catalyzed benzidine rearrangement of bis[4-(2-furyl)-3-methylphenyl]diazane.An example of [9,9]-sigmatropic shift.

정동훈, 박균하

충남대 화학과

Bis[4-(2-furyl)-3-methylphenyl]diazane (1) was prepared by reduction of corresponding bis[4-(2-furyl)-3-methylphenyl]diazene in aqueous acetone solution in the presence of ammonium chloride and zinc. The freshly prepared hydrazo (1) was subjected to acid-catalyzed benzidine rearrangement and we were able to determine the structures of the rearrangement products and their yields quantitatively based on the ^{1}H HMR spectra as shown in the scheme, that is, [9,9]-sigmatropic shift and disproportionation in 40% and 36% respectively. This [9,9]-shift provides another example to our first report on [9,9]-shift.

Scheme



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Synthesis and Characterization of New Anthracene-Based Organic Thin Film Transistor Material

이민정, 배만훈, 박현태, *권순기, 김윤희

*경상대 화학과 *경상대 나노신소재공학부*

Organic semiconductors have a number of advantages over traditional inorganic materials, including chemical tunability, compatibility with plastic substrates and structural flexibility if they can retain high electrical performance. Conjugated oligomers and polymer represent one of the most important classes of advanced materials in recent years. Among the most potential materials for organic semiconductor, thiophene and anthracene based oligomers have received special attentions due to their good electrochemical properties and thermal properties. Here, we designed and synthesized new semiconducting material based on anthrancene.

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Synthesis and Characterization of Blue Organic Luminescenes Material with Limb Structure

배만훈, 이민정, 김윤희, *권순기

*경상대 화학과 *경상대 나노신소재공학부*

현재 Display 분야에서 TFT-LCD 와 OLED 의 세대교체가 이루어지고 있다. LCD 보다 뛰어난 성능과 효율 그리고 잠재력으로 차세대 Display 로써 주목받고 있는 OLED 는 소형 Display 시장에서 이미 상용화가 되었고, 중대형 Display 로 상업화 시키기 위하여 많은 곳에서 연구가 이루어지고 있다. 향후 몇 년 내에는 OLED 가 일상적인 Display 로 등장하게 될 것으로 예상된다. Anthracene 은 OLED 의 발광층의 재료로 많이 사용되는데, Anthracene 을 모체로 하는 많은 청색발광물질은 일반적으로 2 번과 6 번 위치에 많은 치환체들이 도입되고 있다. 본 연구에서는 2 번과 3 번 위치에 Methyl Group 이 포함된 Phenyl 을 도입함으로써 분자간 상호작용이 최대한 억제되어 색순도와 효율이 높은 청색발광재료가 될것으로 예상되는 물질을 합성 및 그 특성을 조사하였다.

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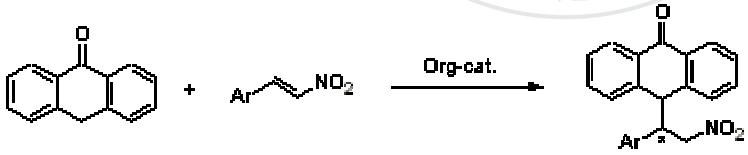
Asymmetric Michael addition of anthrone to nitroalkenes with bifunctional organocatalysts

, 채영미, 강영구,, 김대영,

순천향대 화학과

Anthrone usually functions as a reactive diene in the presence of base and a variety of dienophiles, furnishing the corresponding Diels–Alder reaction products in good yields rather than the Michael adducts. Only in few cases the corresponding Michael adducts were isolated as by-products in Diels–Alder reactions using anthrone.In this presentation, we wish to communicate a novel bifunctional organocatalysts catalyzed enantioselective Michael additions of anthrone. The Michael addition of anthrone with nitroalkenes to give the corresponding Michael adducts in good yields and excellent enantioselectivities in the presence of bifunctional organocatalysts.



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Organocatalytic Enantioselective Michael Reaction of Nitroacetate to α,β-Unsaturated Enones in Water.

문형욱, 김대영

순천향대 화학과

The Michael reaction of carbon nucleophiles to electron-poor alkenes is among the most powerful transformations for the formation of carbon–carbon bonds in organic synthesis. The highly enantioselective Michael reaction of nitroacetate to α,β-unsaturated enones has been developed in water. The Michael adducts could easily undergo a simple denitration or decarboxylation procedure to give the corresponding optically active δ-ketoesters or γ-nitroketones.

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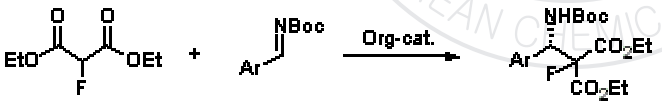
Asymmetric addition reaction of α-fluoro malonate to N-Boc aldimines using bifunctional organocatalysts

윤성제, 강영구, 김대영

순천향대 화학과

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 β-amino acid derivatives. The catalytic enantioselective Mannich reaction promoted by chiral bifunctional organocatalysts is described. The treatment of α-fluoro-malonate with N-Boc-aldimines under mild reaction conditions afforded the corresponding β-amino acid derivatives with excellent enantioselectivities (up to 97% ee).



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Enantioselective Fluorination of α-Chloroketoester Catalyzed by Chiral Nickel Complexes

강승희, 김대영

순천향대 화학과

Fluorine-containing organic molecules are becoming increasingly important in medicinal chemistry. In particular, Very few methods for the preparation of α-chloro-α-fluoro-β-ketoester are known. In this presentation, we wish to communicate the catalytic enantioselective fluorination of α-chloroketoester in the presence of air- and moisture-stable chiral nickel complex. The catalytic elecrophilic fluorination of α-chloroketoester to give the corresponding chiral hetero dihalocompound with excellent enantiomeric excesses (up to 99 % ee).

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발표종류: 포스터, 발표일시: 금 10:30~12:30

Asymmetric organocatalytic aldol reations of α-keto phosphonates with ketones catalyzed by chiral primary amine catalysts

이현주, 강영구, 김대영

순천향대 화학과

Aldol condensation is one of the basic reactions for creating a C-C bond. α-Hydroxyalkyphosphonic acid derivatives is very important because they have been shown enzyme inhibitors. The catalytic enantioselective aldol reaction promoted by a novel primary amine catalyst is described. The treatment of α-keto phosphonates with ketones under mild reaction conditions afforded the corresponding tertiary α-hydroxyalkylphosphonates with moderate enantioselectivities.

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Catalytic enantioselective Friedel-Crafts reaction of indoles with unsaturated keto phosphonate derivatives

권보경, 강영구, 김대영

순천향대 화학과

The Friedel-Crafts reactions are very important and useful for carbon-carbon bond formations. Their catalytic enantioselective reactions have attracted a great deal of recent attention owing to easy access to optically active aryl substituted products from readily available starting materials. In this presentation, we describe the utility of the chiral palladium complexes in the catalyzed additions of indole derivatives to γ,δ-unsaturated β-keto phosphonates and β,γ-unsaturated α-keto phosphonates. Treatment of γ,δ-unsaturated β-keto phosphonates and β,γ-unsaturated α-keto phosphonates with indole derivatives to give corresponding Fridel-Crafts adducts in high yields and enantioselectivities (up to 99% ee).

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A new partial reduction method of tertiary amides to aldehydes

김소영, 안덕근

강원대 화학과

The establishment of a simple, general and practical functional group transformation in one-pot is one of the most important and highly desirable objectives in organic synthesis. Also, synthesis of aldehydes from tertiary amides is valuable synthetic tool, and a large number of partial reducing agents for this purpose have been reported to now. Among them, diisbutylaluminum hydride (DIBALH), which is commercially available, is used as one of the popular reducing agent for this purpose. However, the yields of aldehydes (50-70%) are considerably lower than other useful reducing agents. Now, we wish to introduce new synthetic methodology of aldehydes from tertiary amides is almost quantitative yields using DIBALH.

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Towards Smart Supramolecular Polymers Based on Strong Host-Guest Interactions between Cucurbit[7]uril and Ferrocene

안영주, **N. Selvapalam**, 고영호, 장윤정, *박경민, 김지연, 김기문

*포항공과대 화학과 *포항공과대 첨단재료과학부*

Supramolecular polymers are polymeric arrays of monomer units held together by non-covalent interactions such as hydrogen bond, metal-ligand coordination and host guest interactions. To build useful polymers using non-covalent interactions, the interactions between monomers must be strong and kinetically stable. However, there are few practically useful supramolecular polymers formed in aqueous solution owing to the weak interaction between monomers in water. We therefore decided to develop stimuli-responsive supramolecular polymers prepared in water by taking advantage of the extremely strong host-guest interactions between cucurbit[7]uril (CB[7]) and ferrocenemethylammonium (FA) ion (K ~10^{12}) in aqueous solution. Here, we present our strategy to synthesize the stimuli-responsive supramolecular polymers based on the CB[7]-FA interactions and the synthesis of two interacting monomers, dicucurbit[7]uril(DiCB[7]) and diferrocenemethylammonium (DiFA) composed of two CB[7] and FA units, respectively, linked by a hydrophilic bridge to form a supramolecular polymer in aqueous solution. The details of the synthesis the two monomer units and self-assembly of a supramolecular polymer will be presented.

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Doubly activated coumarin fluorophore as a colorimetric and fluorescent probe for cyanide in water

김건중, 김해조

경기대 이과대학 화학과

A simple aldehyde-functionalized coumarin (1) was utilized as a doubly activated Michael acceptor type of chemodosimeter for cyanide in water. The probe has shown a selective and sensitive response to the cyanide anion over other various anions through the Michael addition reaction of the cyanide to 1. When cyanide anions were added, the prominent color changes as well as the fluorescence changes of 1 were observed so that millimolar concentrations of cyanides were detectable by the naked eye.

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Limb 구조의 Antracene 청색 발광 물질 개발

강소희, 소기호, 박현태, 김윤희, *권순기

*경상대 화학과 *경상대 나노신소재공학부*

오늘날 정보 디스플레이 산업이 발전함에 따라 OLED 는 자체발광, 빠른 응답속도, 넓은 시야각, 얇은 두께, 저 소비전력, 단순한 제작공정 등의 특징으로 디스플레이용 소자로서 각광 받고 있다.국내외 여러회사에서 이미 상용화가 이루어졌으며, 현재 상용화가 이루어지고 있는 유기발광다이오드는 대부분 유기 단분자 재료로 구성되는 적층형 구조로 제작된다.평판 디스플레이의 최종 목적인 풀칼라 구현을 위한 유기발광다이오드를 이용한 방법은 RGB 3 원색의 독립발광에 의한 개별화소 구동방법과 백색발광과 칼라필터에 의한 방법등이 주로 연구 되고 있다.본 연구에서는 Limb 구조의 Antracene 을 이용한 청색 발광 물질을 연구하고 합성하였다.

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Rhodamine-Hydroxylamine-Based Fluorescent Chemosensor for the Detection of Fe(III)

지승희, 문경수, 태진성

연세대 화학과

Iron is widely distributed in nature and is one of the most important elements in biological systems, which plays a crucial roles in many biochemical processes at the cellular metabolisms. Especially, ferric iron Fe(lll) is an essential element for the formation of hemoglobin of red cells and transport of oxygen to tissues and several enzymes contain ferric ions as part of a catalytic site. Most of the known Fe(lll) sensors are based on the fluorescence quenching mechanisms due to the paramagnentic nature of ferric ions. Biological Fe(lll) processes utilize siderophores, such as analogues of ferrichrome or enterobactin which possess either hydroxamates or catecholates as binding sites. Recently, examples employing fluorescent enhancements upon Fe(lll) reversible bindings and irreversible chemical reaction have been reported, but the sensitivity of those fluorescent probes still needs to be improved. Thus, we have demonstrated that a new turn-on fluorescent chemosensors for Fe(lll) based on the aminooxy-linked ethylene glycol binding unit coupled with the rhodamine fluorophore. These chomosensors strongly bind with Fe(lll) induce a large increment in the fluorescence intensity and a marked color change. Importantly, the selectivity and sensitivity of this system for Fe(lll) over other metal ions is extremely high.

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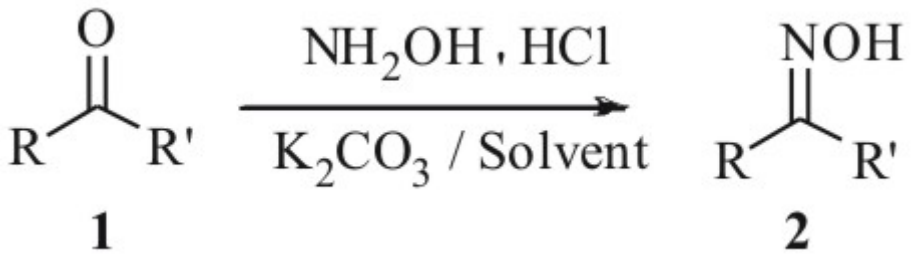
Convenient Synthesis of Oxime

김은정, 이형근, 김보람, 이인혜

경상대 화학과

Oximes are interested class in synthetic chemistry. Although many methods have been reported, known methods have some drawbacks, such as low yields, high reaction temperature, using toxic materials, and long reaction time. In order to solve these problems, we attempt to find an economically and environmentally favored method. Herein, we present novel convenient preparation of oximes under mild conditions.



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Synthesis and anticancer activity of novel amide derivatives of non-acetal deoxoartemisinin

박지현, 이용남, 임은영, 정만길

연세대 화학과

현재까지 다양한 non-acetal deoxoartemisinin 유도체가 합성되었으며 이 유도체들의 항말라리아성에 관한 많은 생리활성연구가 진행되어졌고 보고되었다. 본 연구실에서는 항말라이아성이 아닌 최근 새롭게 보고되고 있는 항암성에 관한 연구를 수행하고 있으며 특히 Antiangiogenic activity 에 관한 연구를 실시하고 있다. Artemisinin 과 Artemisinic acid 로부터 합성된 Deoxoartemisinin 유도체에 대해 CAM assay(Chorioallantoic Membrane assay)와 In Vivo Matrigel Plug assay 를 수행하여 높은 Antiangiogenic activity 를 가지는 것을 확인하였고 이 화합물들이 새로운 항암물질의 가능성을 가지는 것을 발견하였다.

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Direct Amination of Benzoxazoles Under Highly Mild Conditions

김지영, 조승환, 장석복

KAIST 화학과

Transition metal-catalyzed C-N bond formation is highly important in synthetic chemistry since it can offer nitrogen-containing molecules of great interest in biological, pharmaceutical, and materials sciences. Variety of C-N bond forming reactions with organic halides and organometallic compounds are developed. Despite these remarkable progresses, limited examples are shown for C-H functionalization with amines.During our efforts on metal-catalyzed C-H bond functionalization, we found that Ag-mediated C-N bond formation of benzoxazole could be achieved under much milder conditions (60℃) in the presence of acid. However, disadvantage of this reaction was that stoichiometric amount of expensive silver was required.On the basis of the proposed mechanistic consideration, we envisioned that stoichiometric silver could be replaced by other oxidant system. Finally, we found that catalytic amount of other transition metal (eg. Co, Mn, or Fe) with peroxide were employed for this amination reaction at room temperature.

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마찰저감제로 사용하기 위한 Thiocarbamate Dendrimer의 합성과 물성측정

김성기, 김영준

충남대 화학과

본 연구에서는 중금속을 포함하지 않고 마찰저감 효과를 줄 수 있는 thiocarbamate dendrimer 마찰저감 소재를 합성하였다. 덴드리머는 succinic acid 와 glycerol 로 구성되고 말단가지에는 thiocarbamate 그룹이 2, 4, 8, 16 개로 포함된 각각 1, 2, 3, 4 세대를 합성하였다. 합성된 마찰저감 소재의 일정량을 Diester oil(DB-51), 광유계 오일(100N), 식물유(Soybean)에 용해하여 4-ball WSD 시험기로 1200rpm/20kgf 에서 1 시간 측정하여 마찰저감 효과를 측정하였다. 결과는 thiocarbamate 그룹이 많이 함유된 덴드리머일수록 마찰저감 효과가 뛰어난 것으로 관측되었다.

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Highly Efficient Blue Fluorescent OLEDs using Double and Mixed Emission Layer through Pyrene Derivatives

김명기, 홍종인

서울대 화학부

We have synthesized deep blue fluorescent materials for OLEDs comprising pyrene and triphenylamine (PTPA) or pyrene and oxadiazole (PPBD). We tested if the efficiency of blue fluorescent OLEDs can be improved by using double emission layer (DEL) and mixed emission layer (MEL). The DEL and MEL devices show significantly improved quantum efficiency by a factor of 2 and 3 as compared with that of a device using single emission layer (SEL), respectively. The devices based on 5% doped PTPA and PPBD into ADN exhibited an external quantum efficiency of 3.1%, 2.8% with the CIE coordinates at (0.15, 0.09), (0.15, 0.07), respectively. The devices based on 100% PTPA and PPBD exhibited an external quantum efficiency of 1.1%, 1.2% and with the CIE coordinates at (0.15, 0.13), (0.17, 0.20), respectively. Also, DEL and MEL devices show an external quantum efficiency of 2.8%, 3.5% and with the CIE coordinates at (0.15, 0.16), (0.15, 0.19), respectively. Experimental details and mechanisms will be discussed in the presentation.

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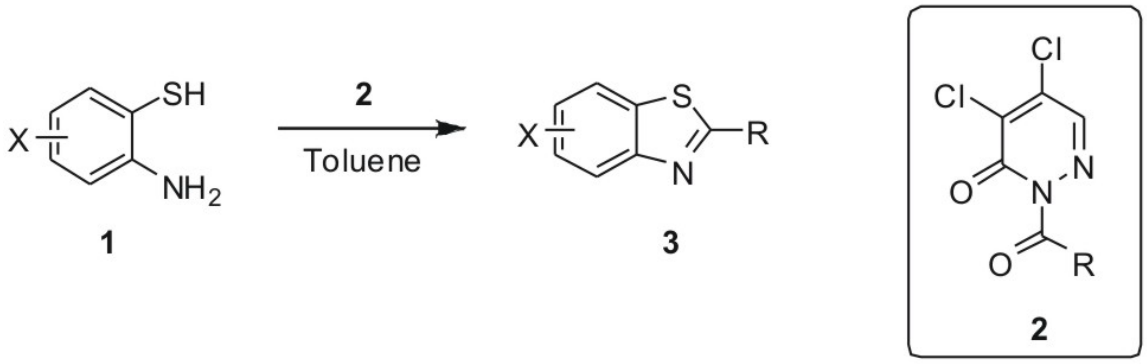
Synthesis of Benzothiazoles Using 2-Acylpyridazine-3(2H)-ones under Neutral Conditions

이인혜, 이형근, 김보람, 김은정

경상대 화학과

Benzothiazoles is very important in medicinal and industrial chemistry due to various biological properties: antiglutamate, antimicrobial, antitumour, antiparkinson, inhibition of enzymes, etc. Although the synthetic methods of benzothiazoles have been reported, these suffer from one or more of the following drawbacks such as strong acidic conditions, expensive catalysts, long reaction times, low yields, tedious work-up and the use of toxic regents. Therefore, we attempted to synthesis of benzothiazoles using 2-acylpyridazine-3(2H)-ones an acyl source under acid-/base-and catalyst-free conditions.Herein, we present novel and convenient synthesis for benzothiazoles using 2-acylpyridazine-3(2H)-ones under neutral conditions.



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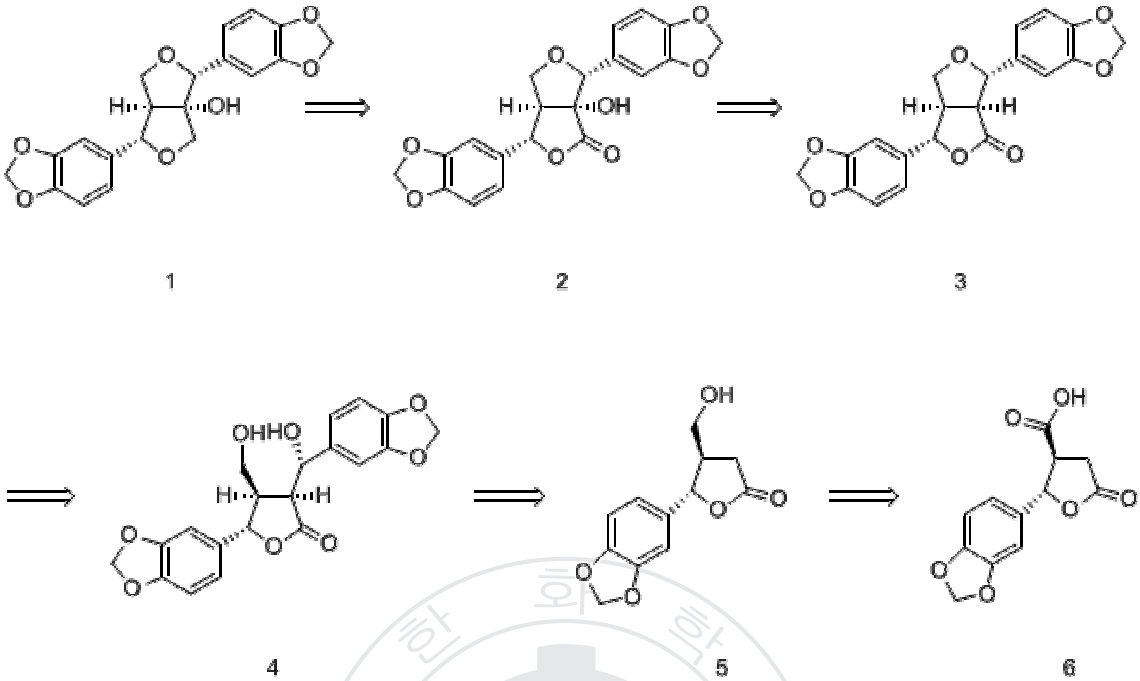
Synthetic Approach For (+)-Paulownin

정선주, 박외숙

충북대 화학과

The goal of this research is to synthesize (+)-Paulownin in its optical active form, which is a symmetrically substituted diequatorial furofuran lignan possessing biologically active properties such as antitumor, antihypertensive and antioxidant. In addition to its useful properties, It has interesting structural features: four continuous stereogenic centers and one tertiary hydroxyl function at the bridgehead carbon C-1.The synthetic method is as follows. S-(-)-4-Benzyl-2-oxazolidinone was deprotonated with n-butyl lithium and reacted with β-carbomethoxy- propionyl chloride to give 1-(4S-benzyl-2-oxazolidin-3-yl)-4 -methoxy-butane-1,4-dione. This 1,4-dione was treated with Ti(O^{i}Pr)Cl3 and DIPEA to form Titanium (Z)-boron enolate which was reacted with piperonal to obtain (2S,3S)-2-piperonyl-5-oxotetrahydrofuran-3-carboxylic acid 6.This acid was reduced with BMS to obtain the corresponding alcohol 5. This alcohol 5 was treated with several base such as LDA, LHMDS, KHMDS and reacted with piperonal to produce the diol-lactone compound 4 in various diasteomeric ratios. this diol-lactone 4 was cyclized to give the compound 3 with MsCl, Et3N and DMAP. The compound 3 was treated with LDA and MoOPH to afford the hydroxylated compound 2. the compound 2 was transformed to the final product, (+)-Paulownin in the usual way which was developed in our laboratory.

Retrosynthetic analysis



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Fluorescent chemosensors for phosphate-containing anions

김훈준, 배세원, 홍종인

서울대 화학부

Fluorescence sensing with small molecular chemosensors is a versatile technique for elucidation of function of various biological substances. We now report a new fluorescent chemosensor for phosphate-containing anions using metal-anion coordination chemistry. The chemosensor is comprised of 2,2´-dipicolylamine-Zn(II) as a binding motif and antracene as a fluorescent signaling unit for phosphate-containing anions. The variation in the fluorescence of the chemosensor is based on a new mechanism, which involves the binding-induced recovery of the conjugated form of the fluorophore from its low fluorescent less-conjugated state.The selectivity and sensitivity of the chemosensor for the detection of phosphate-containing anions can be utilized for various bioanalytical applications such as fluorescence visualization of phosphate-containing anions in living cells.

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마이크로 웨이브와 재사용 가능한 촉매를 이용한 무수숙신산의 합성

김황민, 김영준

충남대 화학과

숙신산으로부터 무수숙신산을 합성하기 위해 촉매로 양이온교환수지의 한 종류인 엠버라이트를 사용하였고, 이소프로페닐아세테이트 용매 하에서 18 시간 동안 환류하여 89% 수득률로 생성물을 얻었다. 마이크로파를 조사해주는 실험조건에서는 반응시간은이 10 분으로 단축되었고, 90%이상의 무수숙신산 생성물을 얻을 수 있었다. 우리는 마이크로파반응의 최적의 조건과 양이온교환수지의 재사용성에 대하여 토론할 것이다.

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A novel and efficient synthetic method of aldehydes from esters

김유리, 안덕근

강원대 화학과

Partial reduction of esters to aldehydes with efficient reducing agents is one of the most important tools in organic synthesis, and a large number of reducing agents for this purpose have been reported. Also, we have reported that a new class of reducing agents prepared from commercially available diisobutylaluminum hydride (DIBALH) showed effective partial reducing characteristics for various esters. However, we want to find the simple and effective methodology for partial reduction of esters to aldehydes without preparing any reducing agents. Recently, we carried out experiences to find simple and effective method for partial reduction of esters under our purpose, as the result, we have found the new one-pot synthetic method of aldehydes from esters in almost quantitative yields using commercial available reagents only.

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Deracemization/Resolution of Chiral α-Amino Acids Using DPA appended Binol Based Metal Complexes as Resolving Reagents

Raju Nandhakumar

이화여대 화학과

Despite the dazzling potential of asymmetric synthesis, resolution of racemates remains the most favorable approach to the large scale preparation of enantiomerically pure compounds. While enzymatic resolution is more economically feasible, it has certain substrate limitations that require the application of a chemical approach via formation of diastereomeric derivatives. In the latter approach, application of a resolving reagent with a stereogenic center is a well-established practical technique. This work demonstrates the separation of enantiomers via formation of diastereomeric derivatives through an imine bond stabilized by Resonance Assisted Hydrogen Bond (RAHB). The present design can be used for both separation of the enantiomers and deracemization of rac-α-amino acids. The synthesis, characterization of the resolving reagents and the resolution of chiral amino acids will be presented.

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Correlation of the rates of solvolysis of phenyl fluorothionoformate and a comparison with phenyl chlorothionoformate solvolysis

최송희, 성미혜, 문두환, 이예린, 경진범

한양대 응용화학과

The specific rates of solvolysis of phenyl fluorothionoformate have been measured at 10.0℃ in a variety of pure and binary solvents. From the specific rates, the sensitivities (*l* and *m*) to changes in solvent nucleophilicity and solvent ionizing power and solvent deuterium isotope effect, k_{MeOH}/k_{MeOD} have been determined at 10.0℃. These give a satisfactory correlation over the full range of solvents when the extended Grunwald-Winstein equation is applied. For several binary solvents, a parallel study was made of phenyl chlorothionoformate solvolysis. These observations are also compared with those previously reported for the corresponding phenyl chloroformate and fluoroformate, and proceeding by an addition-elimination mechanism.

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발표종류: 포스터, 발표일시: 금 10:30~12:30

Synthesis and properties of phosphorescent heterocyclic Ir(III) complexes.

오세환, 염을균

충남대 화학과

Conventional fluorescent OLEDs have low efficiencies and limitation of the practical use in panel display. Cyclometalated Ir(III) complex is typical as a phosphorescent dopant for the high emissive efficiency at room temperature from the triplet metal-to-ligand charge transfer (^{3}MLCT) state. We prepared heteroleptic cyclometalated iridium(III) complexes based on 9-(pyrimidin-2-yl)-9H-carbazole as a main ligand and different ancillary ligand (L^X). All the cyclometalated iridium complexes show orange-red photoluminescence ranged from 590 to 604 nm.

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Rational Approach of a Highly Selective and Sensitive Fluorescent Sensing Ensemble for Discrimination of Pyrophosphate and NTPs

이재한, 박충모, 홍종인

서울대 화학부

Recently, there has been a soaring interest in designing sensors that recognize pyrophosphate anion (PPi). It is because PPi plays an important role in energy transduction in organisms and metabolic processes by participating in enzymatic reactions. For example, PPi is released when nucleotide triphosphate (NTP) is incorporated by a polymerase into a growing DNA or RNA strand. PPi is also released when the second messenger such as cyclic AMP and cyclic GMP is synthesized from NTP.

PPi usually exists in a small amount in the presence of a large amount of NTPs in the aforementioned biological systems. Therefore, in order to achieve real-time monitoring of these enzymatic reactions, we need to develop sensors that can discriminate PPi from NTPs. However, it is still a daunting challenge, because NTPs have the phosphate moiety which is structurally similar to PPi. We designed a new PPi sensing system in which the sensing system shows a large increase in the fluorescence intensity upon binding with PPi, but show relatively weak response when NTPs interact with the sensing system. Our sensing system was successfully used for the monitoring of a polymerase chain reaction. Details of the sensing mechanism and its application to the enzymatic reaction will be discussed in the poster presentation.

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Short and Efficient Synthesis of Cyclopentadithiophene and Its Dialkylated Product

박지혜

아주대 분자과학기술학과

A rapid and efficient synthetic route for cyclopentadithiophene (CDT) and its dialkylated product is reported. Addition of two equivalents of 3-thienyllithium to methyl 2,2,2-trimethoxyacetate and subsequent acidic work-up and saponification affords 2-hydroxy-2,2-di(3-thienyl)acetic acid. Subsequent treatment with polyphosphoric acid results in Nazarov-type cyclization, yielding 4H-cyclopenta[2,1-b;3,4-b']dithiophene-4-carboxylic acid. Subsequent treatment with KOH in dimethylsulfoxide generates a carboxylate anion, which cleanly liberates CO2 gas at room temperature under a vacuum to give a cyclopentadienyl-type anion of CDT. Protonation or direct dialkylation of the anion gives the targeted CDT and its dialkylated product.

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Rationally Designed Fluorescence Turn-On Sensors: A New Design Strategy Based on Orbital Control

정효성, *이진용, 김종승

*고려대 화학과 *성균관대 화학과*

We explore a new strategy in the chemo-sensor field for fluorescence amplification upon binding with metal ions based on controlled participation of the nitrogen lone pair orbital. The basic architecture of the sensor entails a fluorophore, the sp2 hybridized nitrogen lone pair (-C=N-), and a chelator site referred to as the control part. Though nonplanar and nonfluorescent, compound IC1 achieved pseudo planarity from binding with Zn(II) as indicated by the increased fluorescence signal. Its other analogue (IC2), is also planar and not alike IC1-Zn(II), was fluorescent with a lack of binding affinity to metal ions. The time-dependent density functional theory (TDDFT) calculations revealed that the fluorescence amplification was due to the blocking of the nitrogen lone pair orbital; unlikely geometrical rearrangements were insignificant. This could indicate a breakthrough concept in the future design of fluorescent turn-on sensors.

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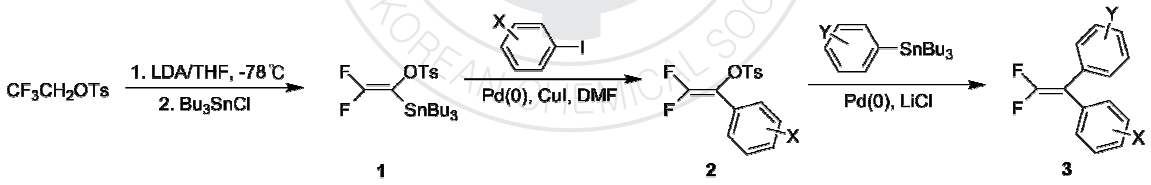
A general and efficient method for the preparation of 2,2-diaryl-1,1-difluoroethenes

한승연, 정인화

연세대 화학및의화학과

β,β-Difluoro-α-tributylstannyl tosylate 1, formed from the reaction of 2,2,2-trifluoroethyl tosylate with 2 equiv of LDA followed by treatment with Bu_3SnCl, underwent the coupling reaction with aryl iodides in the presence of catalytic amount of $Pd(PPh_3)_4$ and CuI to give the coupling products 2 in good yields. The further coupling reactions of 2 with arylstannanes afforded the 2,2-diaryl-1,1-difluoroethenes 3 in good yields. The scopes and limitations of these reactions will be presented.



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Acetone Cyanohydrin as a Practical Source of HCN in the Cu-Catalyzed Hydrocyanation of α-Aryldiazoacetates

박은주, 이승언, 장석복

KAIST 화학과

A new procedure of the Cu-catalyzed hydrocyanation of α-aryldiazoesters has been developed using acetone cyanohydrin as a source of hydrogen cyanide (HCN). It was found that the addition of trimethylsilyl cyanide (TMSCN) significantly accelerates the conversion presumably by delivering free cyanide ion in situ, thus producing various types of α-arylcyanoacetates in high yields under mild conditions.

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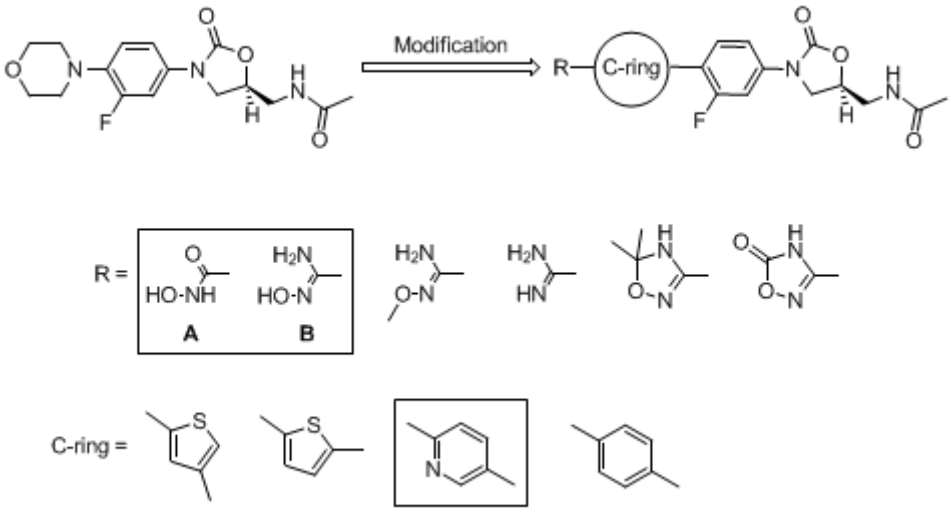
Synthesis of Novel Oxazolidinone Antibiotics

김승태, 윤지훈, 나춘섭, *박규순

*영남대 화학과 *국민대 화학과*

Worldwide spread of multi-drug resistant Gram-positive pathogens led us to develop novel antibiotics. Recently, we synthesized and assayed a series of arylhydroxamides(A) and arylamidoxims(B) which showed highly potent in vitro activities against both Gram-positive and Gram-negative strains including S.aureusMR, S.epidermidisMR, E.faecalisVanA LR, E.faecalisVanA, H.influenzae and M.catarrhalis.Herein we present new oxazolidinone antibiotics including arylhydroxamide and arylamidoxime derivatives and demonstrate in vitro and in vivo assay data in comparison with Linezolid, a representative of oxazolidinone antibiotics.



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Development of Novel ARCA systems for large scale production of D-amino acids

이선민

이화여대 화학 나노과학과

Molecular recognition, especially chiral recognition, is one of the significant processes for diverse chemical and biological phenomena. The study of synthetic modeling systems for chiral recognition of amino alcohols, amino acids and amines is an area of ever increasing research activity. Although much progress has been made, it remains a challenge to develop highly stereoselective receptors for these substrates based on simple organic molecules. In the past years, we developed several binol based receptors for amino alcohols and amino acids called as ARCA systems. On continuation of our work, we report here a novel ARCA receptor which has many advantages such as solubility in organic solvents and high enantioselectivity towards the chiral amino alcohols and amino acids, compared to the other developed receptors. These receptors enantioselectively binds an amino acid and converts L-amino acid to D-amino acid. Hence, D-amino acids can be produced in large scale under operationally convenient conditions without inert atmosphere, rigorously dried/degassed solvents, or difficult-to-maintain temperatures. Furthermore, they are used to enantioselectively recognize various 1,2-amino alcohols. The synthetic details of these receptors, the molecular recognition properties studied by 1H NMR and the production of D-amino acids will be presented.

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Aluminum amide mediated synthesis of oxalyl bis-amide

이영석

대구가톨릭대 화학과

Unsymmetrical oxalyl bisamide are found in many biologically active compounds both synthetic andnatural. In this presentation, the conversion of oxalyl esters into unsymmetrical oxalyl bisamide using thealuminum amide reagents derived from a variety of amine species, including primary, secondary,aliphatic, and aromatic amines will be discussed

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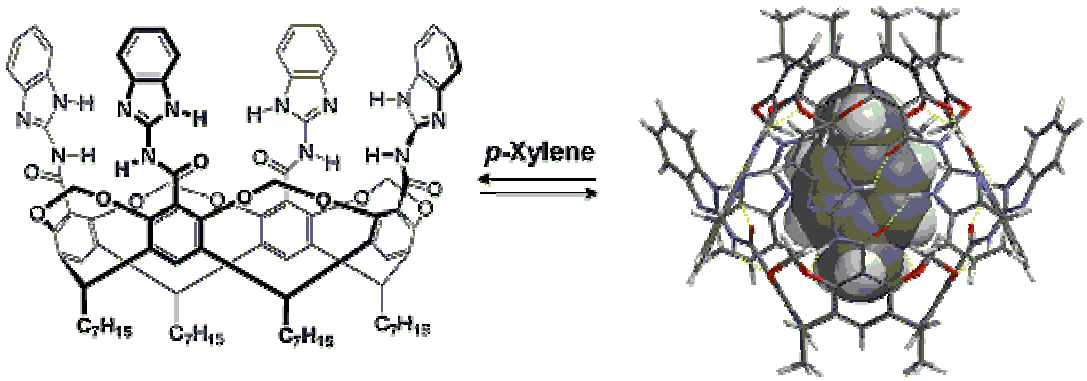
Resorcin[4]arene-Based Molecular Capsules Using Amidobenzimidazole Groups for Hydrogen Bonding

박연실, 백경수

숭실대 화학과

Self-assembling molecular capsules based on noncovalent interactions have attracted considerable interest due to their potential as molecular storage, sensor, catalysts, or reaction chambers in the field of supramolecular chemistry. Cavitands having four amidobenzimidazle moieties on the upper rim of its resorcin[4]arene unit formed stable molecular capsules in nonpolar solvents by the eight intermolecular amide C=O•••H-N benzimidazole hydrogen bondings, two from each four paired amidobenzimidazole, and the four intramolecular O-H_2C-O•••H-N hydrogen bondings on each cavitand. The synthesis and versatile characteristics of these amidobenzimidazole molecular capsules toward anionic, cationic, and neutral guests will be presented.



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A short synthesis and electrochemical characterization of functionalized thieno[3,4-b]thiophenes

정규관, *이화선, **안병준, ***표명호

*전북대 과학교육학부 *전북대 화학교육 **전북대 화학교육과 ***순천대 화학과*

Thieno[3,4-b]thiophene derivatives that have been recently used as monomers of conjugated copolymers for application to polymer solar cells was efficiently synthesized via two steps starting from 3,4-dibromothiophene. The reaction of 3,4-dibromothiophene with an alkyne under Sonogashira condition afforded mono-substituted bromothiophene in good to moderate yields. Anionic substitution and then cyclization of 3-bromo-4-alkynyl substituted thiophene by addition of Na2S gave rise to 2-substituted thieno[3,4-b]thiophene derivatives in moderate yields. Electrochemical polymerization of 2-functionalized thieno[3,4-b]thiophene derivatives gave conjugated polymers in good yields respectively. The polymers showed small bandgaps (□ 0.92 eV) that were measured by oxidation/reduction potentials and NIR spectra of neutral polymers.

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Solid-phase combinatorial synthesis of Quinoxaline library : targeting PTPs

김용진, *이상협

*대구가톨릭대 화학과 *대구가톨릭대 생명화학과*

A combinatorial solid-phase synthesis of Quinoxaline Library is reported.Our research program has centered on the application of polymer-bound α-diazo-β-ketoesters as key building blocks for the solid-phase combinatorial synthesis of a series of heterocycle libraries such as oxazoles, indoles, imidazolones, pyrazinones, etc. We recently discovered that *o*-nitroanilines and *o*-azidoanilines served as excellent substrates in N-H insertion reactions with rhodium carbenoids derived from α-diazo-β-ketoesters. Furthermore, the resin-bound N-H insertion products were then cyclized readily by the treatment of $SnCl_2$ or TPP followed by oxaidant (DDQ, chloranil, etc) to yield the corresponding quinoxalines, which can be further derivatized by a diversity-building, Lewis acid mediated amidation reaction upon cleavage.

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Synthesis of new Ozonides from α,β-Unsaturated 6-Ring Ketones.

liwei, 이은희, 박형진, 구본석, 정인찬

한서대 화학과

For a long time studies concerned with the preparation and properies of ozonides were predominantly of academic interest, since ozonides have found no applications as such, and since they also played only a minor role as supposed or actual intermediates in synthetic reactions or in structural elucidations by their conversion into non-peroxidic products. In resent years, however, a number of naturally occurring organic peroxides have been found to play a role in biochemical reactions. A case in point is the naturally occurring cyclic peroxide artemisinin, which exhibits antimalarial activity. The Synthesis of ozonides could be rationalized by cycloaddition of carbonyl oxide, commonly called criegee-zwitterions and the carbonyl compounds which are derived from the primary ozonide of olefins. Then they get corresponding ozonide by recombination of cycloaddition. A variation of this procedure is the so-called cross-ozonolysis reaction, in which an olefin is ozonized in the presence of an excess of a foreign carbonyl compound to give the cross-ozonide. The structures of all isolated ozonides were established by 1H-NMR and 13C-NMR spectroscopy, and their reduction with triphenylphosphin to give the expected carbonyl compounds.

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Synthesis and Recognition properties of CoumarinCrown Ethers

장승현, 최진욱

대구대 화학과

In this study, we have synthesized the compounds 1～8 from coumarin derivatives which emit fluorescence and crown ethers. To investigate the features of selective recognition by the fluorescence, various cations were added into the compounds synthesized by us. In addition, we performed the experiments which obtain data of the physical properties in order to examine possibility as the fluorescent sensor. Fluorescence spectra of the compounds 1～8 and their reactants were measured with a spectrofluorometer. The reactants could not almost observe fluorescence, while the compounds which are synthesized displayed fluorescence strongly. Measurements of the cation recognition of 15-crown-5 compounds 1～4 containing coumarin by using a spectrofluorometer resulted in decrease of fluorescence intensity about all compounds 1～4 and Na+ showed the best cognitive ability of the measurement results of quantitative recognition. 18-crown-6 compounds 5～8 entirely reduced fluorescence intensity as well and the cognition ability of K+ was the best of several cations. These results informed that the more the coumarins contain the substitution function which has the high electronegativity, the better the compounds have selectivity for the cations.

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Synthesis and Recognition properties of Perylenebis-Crown Ethers

장승현, 최진욱

대구대 화학과

New two host bis-crown ethers containing perylene and naphtalene compounds. Fluorophore containing crown compound was synthesized from 2-(aminomethyl)-15-crown-5, 2-(aminomethyl)-18-crown-6 and 3,4,9,10-perylene tetracarboxylic dianhydride. The other fluorophore Crown ether was prepared 2-(aminomethyl)-15-crown-5, 2-(aminomethyl)-18-crown-6 and 1,4,5,8-naphthalene tetracarboxylic dianhydride. We will also present some of recent recognition results. Binding interaction of the new bis-crown ethers with metal cations was studied through absorption spectroscopy and emission spectroscopy.

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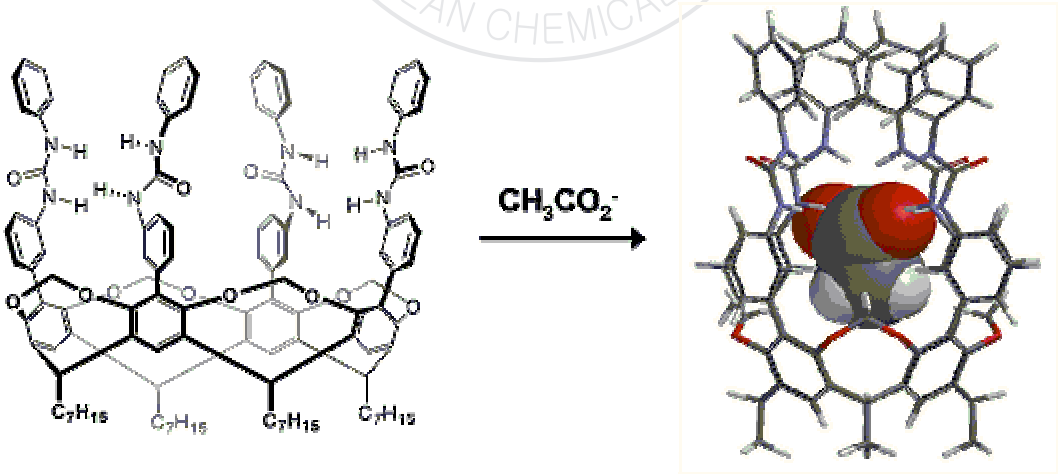
Tetraphenylurea-cavitand for Anion Binding

서성종, 백경수, 박연실

숭실대 화학과

There are currently considerable efforts on exploring efficient artificial receptors for targeted anion recognition and the sensing of anions are ubiquitous and play important roles in biological, medical, environmental, and chemical sciences. We have developed anion sensors by the introduction of four phenylurea moieties on the upper rim of a resorcin[4]arene structure. The binding properties of several anions were investigated in DMSO-d_6 using ^{1}H NMR spectroscopic methods, and the best recognition properties toward carboxylate anions were observed by cavitand 1 through 1:1 host-guest complex formation.



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효소를 촉매로 이용하여 2 가지 상에서 숙신산의 esterification

한상필, 김영준

충남대 화학과

esterification 반응은 물에 대하여 민감한 반응이다. 이런 역반응을 줄여보기 위하여 산촉매를 대신하여 효소를 이용한 반응을 하였다. 지금까지 낮은 온도에서도 쉽게 반응을 할 수 있는 효소를 이용한 esterification 은 많이 실험되고 연구되었다. 그 중에서도 Novozym 435 는 유기용매에서 esterificaiotn 시키는 많이 연구된 효소이다. 이 효소를 이용하여 숙신산과 알코올, 효소의 양은 일정하게 하고 물의 양과 온도의 변화를 주어 반응을 하였다. 그리고 Amberlite XAD 7HP 효소를 이용하여 Nozyme 435 의 반응과 비교하였다.

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Study on Photo-responsiveness of Azobenzene Derivatives Grafted on Silicon Substrates.

민미숙, *유병찬, **이효영

*성균관대 화학과 *목원대 생의약 화학과 **성균관대 화학과, CSMM*

A series of para-substituted azobenzene diazonium salts was efficiently synthesized. Preparation of SAMs on cleaned Si(111) and their characterization by ellipsomery, XPS analyses and contact angle measurements demonstrate formation of a full monolayer on the film. Reversible photo-responsiveness of the solution phase of the azobenzenes upon repeated UV/Vis irradiation was successfully demonstrated according to the UV spectrum analysis. However, their photo-responsiveness on the silicon substrate shows no significant reversible change confirmed by contact angle measurement, indicating that the isomerization on the surface is not as stable as that in their solution phase.A new azobenzene bearing a carbon chain between azobenzene moiety and the metal surface was designed to prevent possible surface quenching during irradiation of the azobenzene SAM on silicon substrate. The methylene-spaced azobenzene was successfully prepared via symmetrical synthetic route from para-nitrophenol followed by asymmetrical addition of nitrosobenzene to the resultant dianiline as the key steps. A full monolayer of the methylene-spaced azobenzene on silicon (111) was realized in acetonitrile (0.15 mM) after 2-3 hr. The SAM was characterized by ellipsomery, XPS analysis and water contact angle measurements. The wettability study by water contact angle measurements upon alternating UV and visible light irradiation demonstrated trans/cis conformational transformation of the methylene-spaced azobenzene in the repeated cycle. The potential applications of such functional hybrid surfaces in microelectronics and molecular electronics can be expected. The subtle structures and quantitative analysis of the modified surfaces will be further investigated.

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발표종류: 포스터, 발표일시: 금 10:30~12:30

Fabrication and modification of biocompatible magnetic nanocrystals for conjugation with cancer-specific targeting

록치충, 채규윤

원광대 화학과

Magnetic colloidal nanocrystals can potentially be utilized as probes and vectors in next-generation diagnosis and therapy. However, the biocompatibility of the magnetic colloidal nanocrystals remains a challenge. In this study, we prepared biocompatible, water-soluble, and superparamagnetic manganese-doped magnetism-engineered iron oxide (MnMEIO) nanocrystals with reactive moieties. We demonstrated that the nanocrystals were not significantly toxic and hence are biocompatible. These exploratory studies suggest that this high-quality biocompatible magnetic nano-platform can potentially be developed for application in MR imaging and drug delivery systems.

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Synthesis and physical properties of acylated chitin derivatives

Lok Ranjan Bhatt, 안채영, 남선미, 채규윤

원광대 화학과

Chitin, a linear polymer of N-acetylglucosamine is a natural polysaccharide with unique biological and chemical characteristics and wide range application possibilities. Acylation of chitin is one of the methods to improve its solubility. In this study a series of chitin cycloesters were synthesized using cyclocarboxylic acids and Trifluoroacetic anhydride. Prepared chitin esters were characterized using FT-IR and 1H NMR and their thermal property and morphology were analyzed using, differential scanning calorimetry and scanning electron microscopy respectively. The results showed that combining carboxylic acid(s) with chitin provides a new copolymer(s) with improved physical properties including solubility.

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Selective esterification of glucosamine

남선미, *김보미, 채규윤

*원광대 화학과 *원광대 생명나노 화학과*

Selective N-arylation of glucosamine was performed via a Schiff bases formed by the reaction between the 2-amino group of glucosamine with an aromatic aldehyde under acidic condition. This was followed by the acylation of above product in a pre-mixed solution of trifluoroacetic anhydride and carboxylic acid which was heated at 70℃ with mechanical stirring. The ester derivatives of glucosamine were synthesised between glucosamine and various carboxylic acid derivatives in presence of trifluoroacetic anhydrideKeywords : glucosamine, acylation

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Preparation and physical characteristic of chitosan ester derivatives

안채영, 김보미, 이영행, 채규윤

원광대 화학과

Chitosan, a linear polymer of N-acetylglucosamine is a natural polysaccharide with unique biological and chemical characteristics and wide range application possibilities. Acylation of chitosan is one of the methods to improve its solubility. In this study a series of chitosan esters were synthesized using carboxylic acids and Trifluoroacetic anhydride. Prepared chitosan esters were characterized using FT-IR and 1H NMR and their thermal property and morphology were analyzed using, differential scanning calorimetry and scanning electron microscopy respectively. The results showed that combining carboxylic acid(s) with chitosan provides a new copolymer(s) with improved physical properties including solubility.

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Blue Organic Light-Emitting Diodes Based on Spirobifulorene derivatives

이금희, 김슬옹, 윤승수

성균관대 화학과

Organic light-emitting diodes (OLEDs) have been developed for full color displays. But they still need doing more efficient blue-light-emitting materials due to their potential application. In this study, a series of blue fluorescent emitters based on spirofluorene were synthesized via the Horner-Wadsworth-Emmons reaction in moderate yield and their electroluminescent properties investigated. To explore the electroluminescent properties of these materials, multilayered OLEDs were fabricated into a device structure of: ITO / DNTPD (600 Å) / NPB (300 Å) / MADN: Blue dopant materials 1 – 5 (wt %) (300 Å) / Alq_3 (200 Å) / Liq (10 Å) / Al (1000 Å). Among the devices, one device exhibited highly efficient blue emission with a respective luminous, power, and quantum efficiencies of 5.33 cd/A, 2.47 lm/W, and 4.17 % at 20 mA/cm^2. The peak wavelength of the electroluminescence (EL) was 473 nm with CIEx,y coordinates of (0.150, 0.181) at 8.0 V. In addition, a deep blue device with CIEx,y coordinates of (0.150, 0.119) at 8.0 V showed a luminous efficiency of 1.79 cd/A and quantum efficiency of 1.93 % at 20 mA/cm^2.

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Synthesis and Electroluminescent Properties of Chromene Derivatives for Red Fluorescent OLEDs

박민혜, 이금희, 윤승수, *김영관

*성균관대 화학과 *홍익대 기초과학과*

Over the past decade, organic light-emitting diodes (OLEDs) have been rapid progress owing to their potential applications in flat-panel-display technology. In this paper, we reported the synthesis and electroluminescent properties of chromene derivatives for red fluorescent OLEDs. Among OLED devices using these materials as dopants in the emitting layer, a device exhibited efficient red emission with the maximum luminance of 1454 cd/m^2 at 12.0 V. The luminous efficiency, power efficiency and quantum efficiency were 0.75 cd/A, 0.31 lm/W and 1.15 % at 20 mA/cm^2, respectively. The peak wavelength of the electroluminescence was 679 nm with the CIE coordinates of (x=0.62, y=0.34) at 7.0 V.

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Diversity-Oriented-Synthesis of Fluorescent Sensors for Transition Metal Catalysts

YU SUH YOUNG, 홍종인

서울대 화학부

Transition metals such as palladium(II), platinum(IV) and gold(III) play important roles in materials and chemistry. In particular, Buchwald–Hartwig, Heck, Sonogashira, and Suzuki–Miyaura reactions catalyzed by these transition metals have been used for the formation of various covalent bonds. These metal catalysts are being frequently used in the synthesis of various pharmaceutical products. However, even after rigorous purification, residual transition metal catalysts are often found in commercial drugs, which may cause a crucial health hazardous problem. Recently, Koide et al. have developed fluorescent sensors for palladium(II), platinum(IV) by using allylic oxidative insertion reaction. However, these sensors showed fluorescence enhancement merely at the same wavelength as transition metal catalyzed the reactions. Further, we found that the O-allylic bond was easily decomposed at high temperatures without transition metal catalysts. Herein, we report new ratiometric fluorescent sensors for transition metal ions that were developed through diversity-oriented synthesis of fluorescent library approach (DOFLA). Our sensors show distinct fluorescent shift after reaction of the sensors with transition metal catalysts.

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BODIPY-Hexaphyrin Hybrids

신지영, Q. Miao, D. Dolphin, *T. Tanaka, *A. Osuka

*Department of Chemistry, University of British Columbia *Department of Chemistry, Kyoto University*

Currently, expanded porphyrins have emerged as a promising class of molecules in light of their interesting structural, electronic, and coordination properties. Borondipyrromethenedifluoride(BODIPY) have been also widely studied as a class of the efficient energy harvesters and linked to other moieties to prepare diverse hybrids. Herein, we prepared facile BODIPY-hexaphyrin hybrids and determined the light-induced energy transfers from hexaphyrin moiety to BODIPY corresponding temperature-dependent conformational dynamics of hexaphyrin group at low temperature. In all case, efficient intramolecular excitation energy transfers were observed. While [26]hexaphyrin hybrids were considered as an energy transfer from the BODIPY to Hückel aromatic [26]hexaphyrin, [28]hexaphyrin hybrids were considered as the energy transfers onto a Möbius aromatic [28]hexaphyrin. It is to be noted as the firest example of the intramolecular energy transfer involving a Möbius aromatic molecular part as the energy acceptor.

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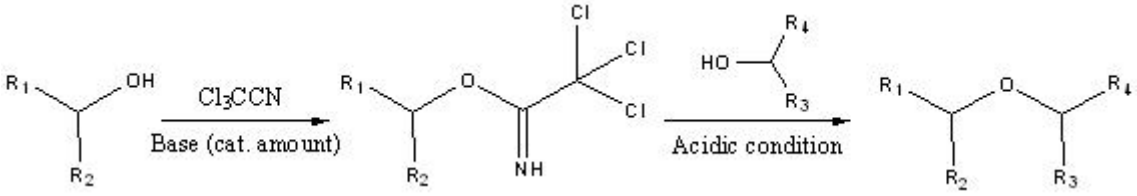
An efficient method for the ether formation using trichloroacetimidates under the acidic condition

김수정, *박훈규, *김학원

*경희대 화학 및 신소재과학 *경희대 화학과*

Williamson ether synthesis is still extensively used for the ether bond formation. However, there are some difficulties for making an ether compound with sterically hindered or base-sensitive alcohols due to its SN2 reaction condition or basic condition. Therefore, we have studied the mild and efficient etherification using trichloroacetimidates under the acidic condition.



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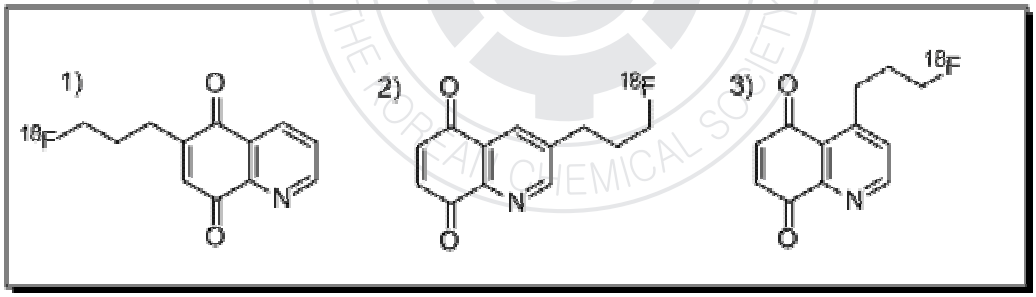
An Efficient Synthesis of (Fluoropropyl)quinoline-5,8-dione for Labeling with Fluoride-18

kalme sachin, 장승호, 박주영, 김동욱

전북대 핵의학과

Various quinoline-5,8-dione derivatives for the development of anticancer agents have been synthesized. To develop positron emission tomography (PET) tracer of these derivatives, we designed several F-18 labeled fluoropropyl quinoline-5,8-dione derivatives at C3, C4, and C6 position have been prepared.



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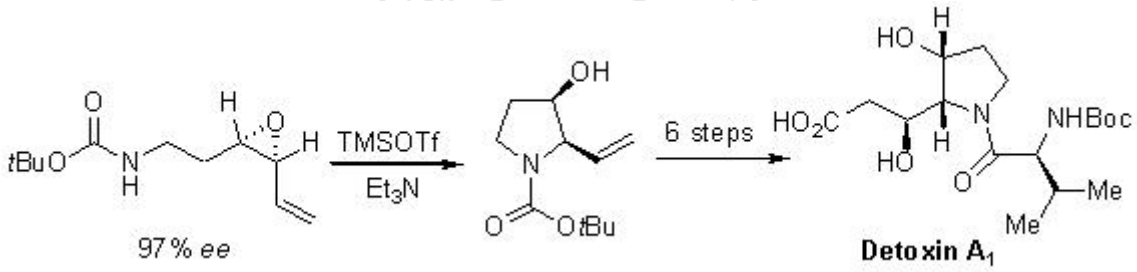
Enantioselective Synthesis of Detoxine A via Diastereoselective Endo-cyclization of Vinyloxiranes

성원제, 유범선, 유찬모

성균관대 화학과

The availability of efficient synthetic methods for achieving absolute stereoselectivity via catalytic process in the production of enantiomerically pure compounds is of considerable current interest in the field of synthetic chemistry. We would like to present herein several crucial points that have emerged from our recent investigations: 1) new method for the preparation of functional allylic boranes from reaction of a sulfur ylide with chiral boranes 2) enantio- and diastereoselective synthesis of 3-vinyloxiranes in high levels of stereoselectivity 3) synthetic applications to the piperidine alkaloids.



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A preparative and spectroscopic study of some phenol-2-thiazole fluorophores for cation detection

Aasif Helal, 김상현, 김현곤, 김홍석

경북대 응용화학과

Preparative and photophysical studies of different phenol-2-thiazole fluorophores with different substituents at the 4 position of the thiazole ring for the detection of cations were carried. The absorption and the emission results show that the fluorescence is produced by the cation induced inhibition of the excited state intramolecular proton transfer (ESIPT) between the phenol and thiazole moieties. The substituents at the 4 position of the thiazole ring produce selectivity and ratiometric behavior of the sensor with different cations.

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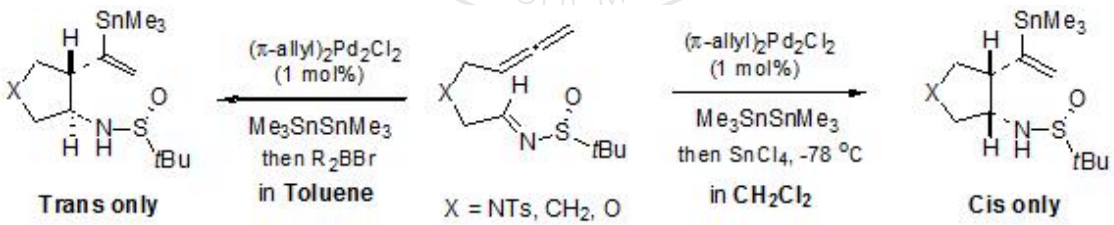
Asymmetric Carbocyclization of Allene-Sulfinimines through Intramolecular Allylic Transfer via Palladium Catalysis

유범선, 양대석, 이민경, 유찬모

성균관대 화학과

The construction of cyclic compounds via organotransition metal catalysts with reagents is of considerable current interest in organic chemistry. This highly stereocontrolled transformation involves the distannylation of an allene moity by palladium catalyst, the transmetallation of the allylstannyl moiety to titanium species, and subsequent the intramolecular allylic transfer reaction to the C=N bond. We wish to present our discovery of a remarkable substrate effect as introduction of the chiral sulfinimine functionality for the cyclization, which allows the reaction process in good yield with excellent diastereoselectivity.



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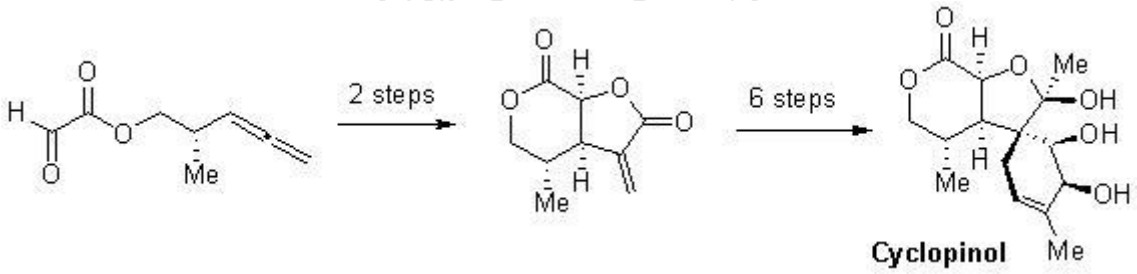
A New Allylic Transfer Reaction of Allenyl-glyoxylates Catalyzed by Palladium Complex: Synthesis of Cyclopinol

양대석, 이보빈, 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. We would like to present herein several crucial points that have emerged from our recent investigations: 1) novel cyclization of allene-glyoxyaldehydes mediated by Pd or Ru complex to afford the bicyclic lactones; 2) synthetic studies toward an enantioselective synthesis of isocyclocalopin A.



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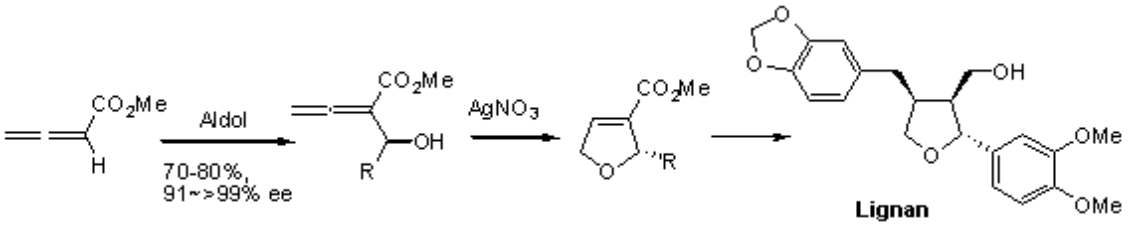
A Highly Enantioselective Aldol Reaction of Allenoates: Synthesis of Lignans

이보빈, 성원제, 유찬모

성균관대 화학과

The availability of efficient synthetic methods for achieving absolute stereoselectivity via catalytic process in the production of enantiomerically pure compounds is of considerable current interest in the field of synthetic chemistry. 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) an aldol condensation of allenoate with aldehyde in the presence of chiral boron bromide 2) Synthesis of dihydrofurans. Stereoselectivity and mechanistic details will be presented.



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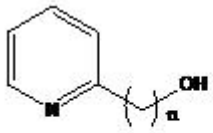
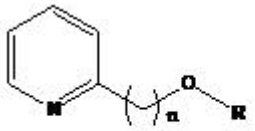
Synthesis and CO2-solubility of 2-substituted pyridine derivatives

임병조, *권현지, 고미선, 김학원

*경희대 화학과 *경희대 응용화학과*

본 발표에서는 Supercritical-CO2 상에서 금속을 추출할 수 있는 친이산화탄소성킬레이트 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 을 도입하여 다양한 2-pyridinealkyl ester 를 합성하였고, 이의 CO2-solubility 를 측정, 비교하였다.





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Stereoselective Synthesis of 2,4,6-Trisubstituted Tetrahydropyrans via Prins-type cyclization

김영습, *이재균, *조용서, *배애님, 최기항, *민선준

*고려대 화학과 *KIST 생명보건본부 뇌의약센터*

Functionalized oxacyclic compounds such as tetrahydrofurans or tetrahydropyrans constitute key structural motifs of a large number of biologically active natural products. One of the efficient synthetic strategies to synthesize these types of heterocycles is Prins cyclization methodology, that is, an intramolecular electrophilic addition of double bond to oxocarbenium ion intermediate.We here report a novel stereoselective synthesis of 2,4,6-trisubstitued tetrahydropyrans having aldehyde functionality at the C4 position via acid-promoted Prins-type cyclization of 2-methylene-1,4-diols with a broad range of aldehydes and acetals. In this study, we will highlight the opportunities in ring construction provided by employing a 1,2-hydride migration to terminate a Prins cyclization.

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Synthesis and Properties of organic dye based on 2,7-disubstituted carbazole donor for efficient Dye-sensitized Solar Cells

이우철, *조나라, *고재중, **홍종인

*서울대 화학 *고려대 소재화학과 **서울대 화학부*

Dye-sensitized solar cells (DSCs) have attracted a great deal of attention due to their low production cost of electricity and relatively high energy conversion efficiency. Photo-sensitizers certainly play a key role for highly efficient DSCs. Ruthenium-based sensitizers, such as N3, N719 and black dye, have achieved efficiencies of up to ~11% under 1.5 G irradiation. In addition, high molar extinction coefficients of metal-free organic dyes allow the use of thinner TiO2 films. Efficiencies of ~9% have been recorded for DSCs using metal-free sensitizer. In this presentation, we synthesized and characterized five organic dyes based on 2,7-disubstituted carbazole. These dyes have high molar extinction coefficients and proper energy level for electron transfer from electrolyte to nanocrystalline TiO2 particle. The best performance was 7.48% in the case of carbazole-derived organic dyes having the largest conjugation length donor and bridging group.

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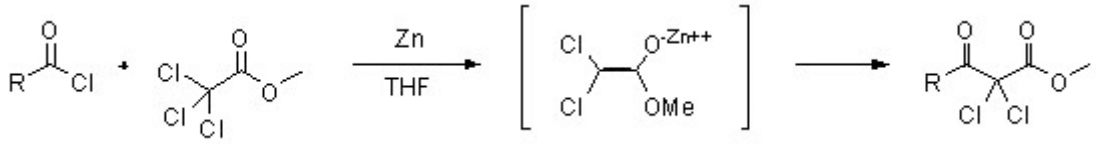
발표종류: 포스터, 발표일시: 금 10:30~12:30

Zn(0)-Mediated Synthesis of Dichloro-Substituted Esters From Carbonyl chloride compounds

최경민

창원대 화학과

Zn(0) was investigated as a cost-effective, environmentally friendly alternative to Cr(II) for the condensation of carbonyls by activated polyhalides.Dichloro-Substituted Esters was synthesized in good yield with method based on Zn(0)-Mediated condensation reaction of a wide variety of carbonyl chloride compounds utilizing commercial methyl trichloroacetate.



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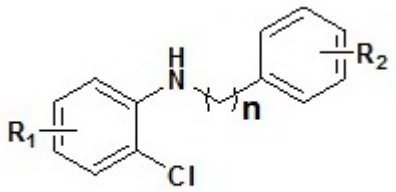
Facile C-N bond formation via Smile rearrangement

최경민, 이상길, 공춘호, 신동수

창원대 화학과

Conventional C-N bond-forming reactions are usually performed via cross-linking of heteroaryl halides with amines, assisted by metal catalysts. We developed one-pot synthesis of diarylamine and arylalkylamine derivatives, simple C-N bond formation via Smiles rearrangement reaction.



R_1 = H, F, methyl,
R_2 = H, methyl, methoxy
n = 0, 1, 2

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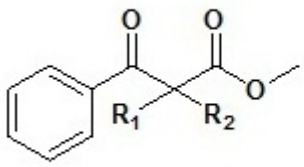
Metal-mediated condensation of acyl halides with methyl trichloroacetate

최경민, 이상길, 정해동, 신동수

창원대 화학과

Methyl 2,2-dichloro-3-oxo-3-phenylpropanoate (1), methyl 2-chloro-3-oxo-3-phenylpropanoate (2), methyl 3-oxo-3-phenylpropanoate (3) were prepared by the reaction of benzoyl chloride with methyl 1,1,1-trichloro acetate using metal-mediated condensation. The more detailed reaction methodology will be discussed



1 : $R_1 = R_2 = Cl$
2 : $R_1 = H, R_2 = Cl$
3 : $R_1 = R_2 = H$

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Probing the diverse DNA structures using end-stacking ability

이일준, 이정우, 김병현

포항공과대 화학과

Constructing and understanding the functions of biomaterials—DNA, RNA, and proteins—are becoming hot research topics in contemporary science. Especially, monitoring the structural states of the biomolecules in solution phase is important for the understanding of their biological functions. Because noncovalent interactions between aromatic molecules are often important for stabilizing the structures formed from biological molecules, we have synthesized and applied various fluorescent nucleoside derivatives for probing secondary structures of nucleic acid. In oligodeoxynucleotides, not only the stacking between DNA bases but the interaction between the fluorophore and DNA base induce the stable form and make possible of the monitoring the conformational diversity of DNA. By recognizing the interaction between DNA bases and fluorophores and using quencher-free molecular beacon concept[1], we could design and synthesize various fluorescent oligodeoxynucleotide systems for monitoring various DNA secondary structures, such as B-Z transition[2], G-quadruplex structures[3, 4] and DNA i-motif structures[5]. 1 (a) Hwang, G. T.; Seo, Y. J.; Kim, B. H. J. Am. Chem. Soc. 2004, 126, 6528. (b) Seo, Y. J.; Ryu, J. H.; Kim, B. H. Org. Lett. 2005, 7, 4931. (c) Venkatesan, N.; Seo, Y. J.; Kim, B. H. Chem. Soc. Rev. 2008, 37, 648.2 Seo, Y. J.; Kim, B. H. Chem. Commun. 2006, 150.3 Seo, Y. J.; Lee, I. J.; Yi, J. W.; Kim, B. H. Chem. Commun. 2007, 2817.4 Seo, Y. J.; Lee, I. J.; Kim, B. H. Bioorg. Med. Chem. Lett. 2008, 18, 3910.5 Lee, I. J.; Yi, J. W.; Kim, B. H. Chem. Commun. 2009, 5383.

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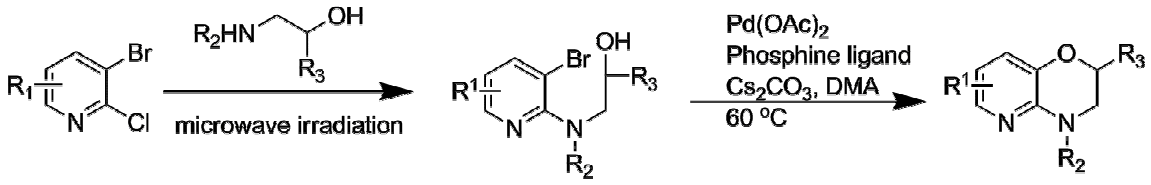
Synthesis of Pyrido[3,2-b][1,4]oxazines via Palladium-catalyzed Intramolecular Cyclization of Aminonoalcohol-tethered 3-bromopyridines.

김정근, *윤우섭, **양은혜, 하덕찬, **하재두

*고려대 화학과 *레고캠바이오 화학과 **한국화학연구원 난치성질환치료제연구센터*

In the course of our research on the synthesis of tyrosine kinase inhibitors, we investigated the utility of palladium chemistry in the synthesis of 3,4-dihydro-2H-pyrido[3,2-b][1,4]oxazines, which 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. For obtaining key intermediates, 2-(3-bromopyridine-2-ylamino)alcohols, a rapid nucleophilic substitution reaction of 3-bromo-2-chloropyridine with various aminoalcohols under microwave irradiation is described. Using this method, the desired products were obtained with the yields up to 70%. Herein we report our efficient method for the synthesis of 3,4-dihydro-2H-pyrido[3,2-b][1,4]oxazine derivatives and their optically pure forms via palladium-catalyzed cyclization reaction of aminoalcohol-tethered 3-bromopyridines.



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Fluoride-selective dosimetric gelator system showing dual optical response in aqueous solution

장동학, 홍종인

서울대 화학부

Recently, many researchers have paid a great deal of attention to the effect of anions on the properties of supramolecular gels. Especially, fluoride responsive gels are reported because of the biological importance of fluoride, such as preventing dental caries and medical treatment of osteoporosis. However, previously reported fluoride-responsive gelators have poor selectivity over other anions. We have developed “dosimetric gelators” which are selectively deprotected by fluoride anions. These deprotection reactions by fluoride not only induced gelation, but also led to fluorescence enhancement. Details of gelation behavior and optical changes upon treatment with fluoride will be discussed in the poster presentation.

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Synthesis and Optical Properties of Dibenzothiophene moiety for Organic Light Emitting Materials

박영진, 김인태

광운대 화학과

Recentyl, a novel materials from dibenzothiophene-S,S-dioxide moiety for OLED have been designed and synthesized. Then we introduced alkyl group containing oxygen for solubility and electron donating group and introduced fluoro for electron withdrawing effects. We were successfully synthesized from diarylamine derivatives by Pd-cat C-N coupling and Stille's cross coupling reaction to good yields. The structure of the resulting compounds were characterized by ^{1}H NMR, ^{13}C NMR, and FT-IR. The optical property and electronic property of the resulting compounds were measured by UV-vis spectroscopy and cyclovoltammetry, respectively.The new materials will be applied to OLED as emitting material.

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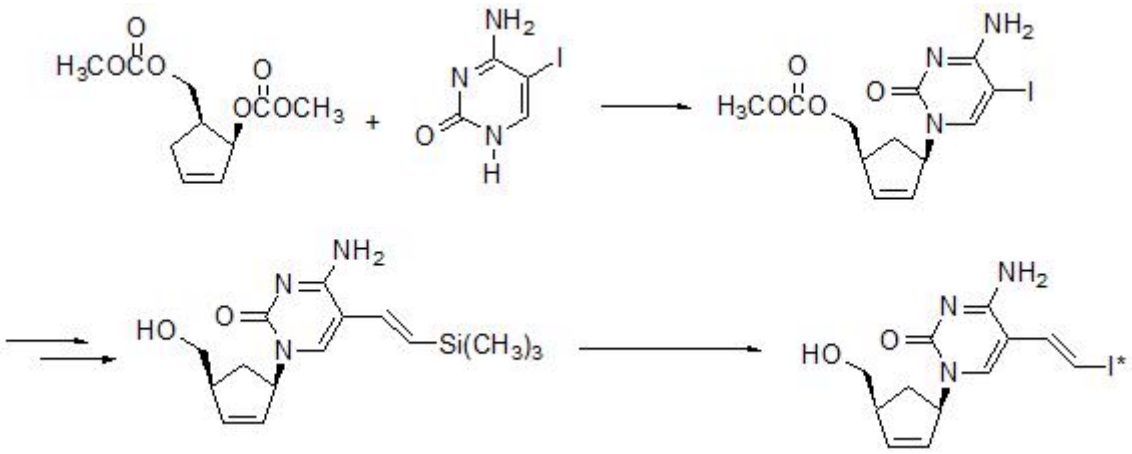
Synthesis of cis-1-[4-(Hydroxymethyl)-2-cyclopenten-1-yl]-5-[124I]iodovinylcytosine(d4IVC): A New Potential PET Imaging Agent for HSV1-TK Expression

안현석, *안광일, 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. Radioiodinated 1-[4´-(hydroxymethyl)-cyclopent-2´-enyl]-5-iodovinyluracil(d4IVC) was synthesized. The synthetic route employed cyclopentadiene as a starting material and proceed in good yield through 8 steps which contain Pd(0)-catalyzed coupling reaction and radioiodination as key reactions. 1-[4´-(Hydroxymethyl)-cyclopent-2´-enyl]-5-iodovinylcytosine was radioiodinated with I-124 using trialkylsilane precursor.



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The study of Anthracenene Dimer with Phosphonium Derivatives

여형민, 전남중, 남계춘

전남대 화학과

Anthracene has the ability to photodimerize with irradiation by UV light. This results in considerable changes in the physical properties of the material. The dimer is connected by two covalent bonds resulting from the [4+4] cycloaddition. The dimer reverts to anthracene thermally or with UV irradiation below 300 nm. The reversible bonding and photochromic properties of anthracenes is the basis of many potential applications using poly and monosubstituted anthracene derivatives. Anthracene dimer was formed ,when phosphonium derivative was treated with excess tetrabutylammonium fluoride. The formed of anthracene dimer confirmed X-ray.

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Au- and Cu-catalyzed Cyclization of Vinyl Allenols

박애리, 신두섭, 이필호

강원대 화학과

Furans and partially reduced furans constitute a large class of naturally occurring compounds that found in a variety of commercially important pharmaceuticals, as well as in flavor and fragrance additives. Consequently, efficient syntheses of such compounds have attracted considerable interest from organic chemists. The functionalized allenyl alcohols were obtained from the reaction of aldehydes with organoindium reagents generated in situ from indium and 5-bromopent-1-en-3-yne. Treatment of allenyl alcohols with gold and copper-catalyst gave rise to 2,5-dihydrofuran derivatives in good to excellent yields.

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Preperation of Rotaxane and Catenane with Non-Covalent Bonding Interaction

전남중, 여형민, 남계춘

전남대 화학과

Topological molecules, catenanes, rotaxanes, knots constitute a major research field in supramolecular chemistry. A number of these multicomponent systems have been named 'molecular machines'. The electron deficient and electron rich components are arranged so that π-π stacking is possible. Our approach has been to bring together neutral marcrocyclic component and containing positively charged ammonium salt to create rotaxane and catenane. The rotaxane and cateanane binding properties investigated with ^{1}H-NMR and fluorescence titration methods with various anions.

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Synthesis of BODIPY-Nucleosides conjugate for Quencher-free Molecular Beacon

김기태

포항공과대 화학과

DNA sequence detection has become important tool for monitoring many biological processes and for other biotechnological applications. One of detection methods is molecular beacon (MB) which can recognize specific target oligonucleotide(ODN) and signal the recognition result by fluorescence intensity. Furthermore, Quencher-free molecular beacon (Qf-MB) containing only fluorophore is developed to enhance efficiency1. Even if QF-MB is economically efficient, it is hard to enhance the signal to noise ratio. Therefore, to improve this, it is important to develop appropriate fluorophore which is sensitive to structure of oligonucleotide and local microenvironments for Qf-MB. Herein, we chose three ethynyl-BODIPY derivatives as fluorophore(fig 1.) because it has good quantum yield, sensitivity to nucleic acid hybridization. BODIPY derivatives are synthesized and can be introduced into nucleoside by sonogashira coupling. Finally, we can also incorporate these nucleosides into QF-MB oligonucleotide and check their ability as reporter probes.

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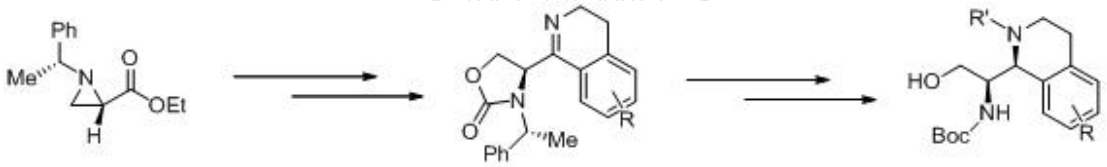
An Efficient Synthesis of Enantiomerically Pure 1,2,3,4-tetrahydroisoquinolines derived Containing β-amino scaffold from a chiral aziridine

이상빈, 이백경, 이규명, 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 nitrogen of 1,2,3,4-tetrahydroisoquinoline after stereoselective reduction of the imine.



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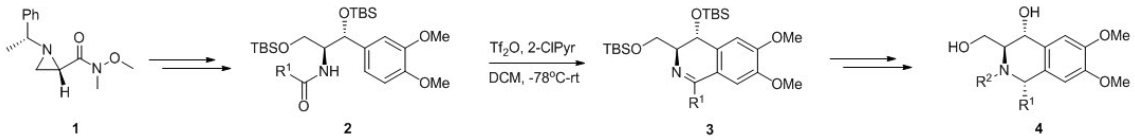
Asymmetric Synthesis of 1,2,3,4-tetrahydroisoquinolines from chiral aziridine

김종찬, 강경연, 김준희, 이원구, *하현준

*서강대 화학과 *한국외국어대 화학과*

The Bischler-Napieralski cyclization of chiral (3,4-dimethoxyphenylethyl)amide initiators 2 derived from (S)-N-methoxy-N-methyl-1-[(R)-1-phenylethyl]aziridine-2-carboxamide 1 is an effective method for the synthesis of 3-hydroxymethyltetrahydroisoquinolin-4-ols, which attract interests from chemists due to their biological activities. Stereoselective reduction of the imine product 3 resulted in (1S,3S,4R)-4-(tert-butyldimethylsilyloxy)-3-[(tert-butyldimethylsilyloxy)methyl]-6,7-dimethoxy-1-methyl-1,2,3,4-tetrahydroisoquinolines 4 in high yield.



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Synthesis of 4-thiazolyl-2-phenylaminopyrimidines

이광무, 김현석, 이필호

강원대 화학과

Heteroaromatic molecules are pharmaceutically important scaffolds, widely found in naturally occurring, as well as synthetic biologically active, molecules. Especially, pyrimidine derivatives are widespread in medicinal and natural product chemistry. A number of commercially important drugs incorporate this heterocycle. Specifically substituted pyrimidines are valuable intermediates for drug discovery. 4-Thiazolyl-2-phenylaminopyrimidines of the pyrimidine derivative is known as a Spleen tyrosine kinase inhibitor. This poster describes synthetic method of 4-thiazolyl-2-phenylaminopyrimidines as a Spleen tyrosine kinase inhibitor.

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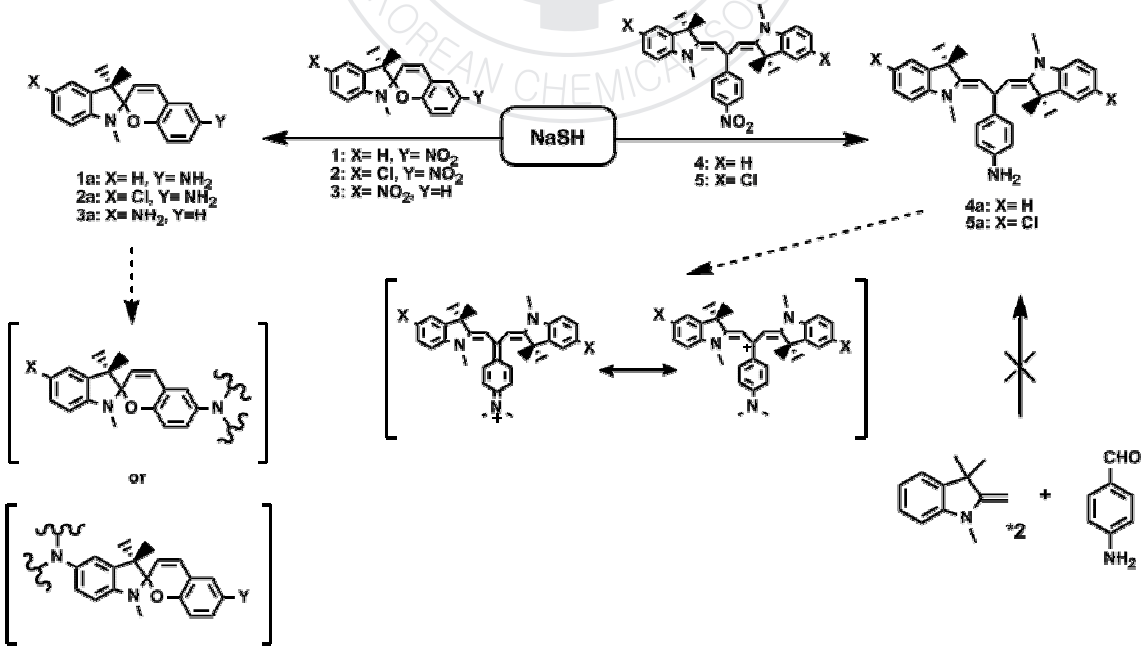
Reduction of spiropyran nitro-derivatives and nitro leuco-TAM dyes with sodium hydrosulfide in ethanol

마소영, *금삼록

*고려대 소재화학과 *고려대 소재화학과*

The target amino-molecules were successfully prepared from the reaction of spiropyran nitro-derivatives (1-3) or nitro leuco-TAM dye (4-5), refulxing with sodium hydrosulfide in ethanol for 5~6 hrs. This method is very simple and in high-yield, compared to the traditional reduction with tin(II) chloride. The prepared amino-molecules (1a-5a) were characterized by ^{1}H NMR, ^{1}H -^{1}H COSY, ^{13}C NMR, UV-Vis and IR spectroscopy.



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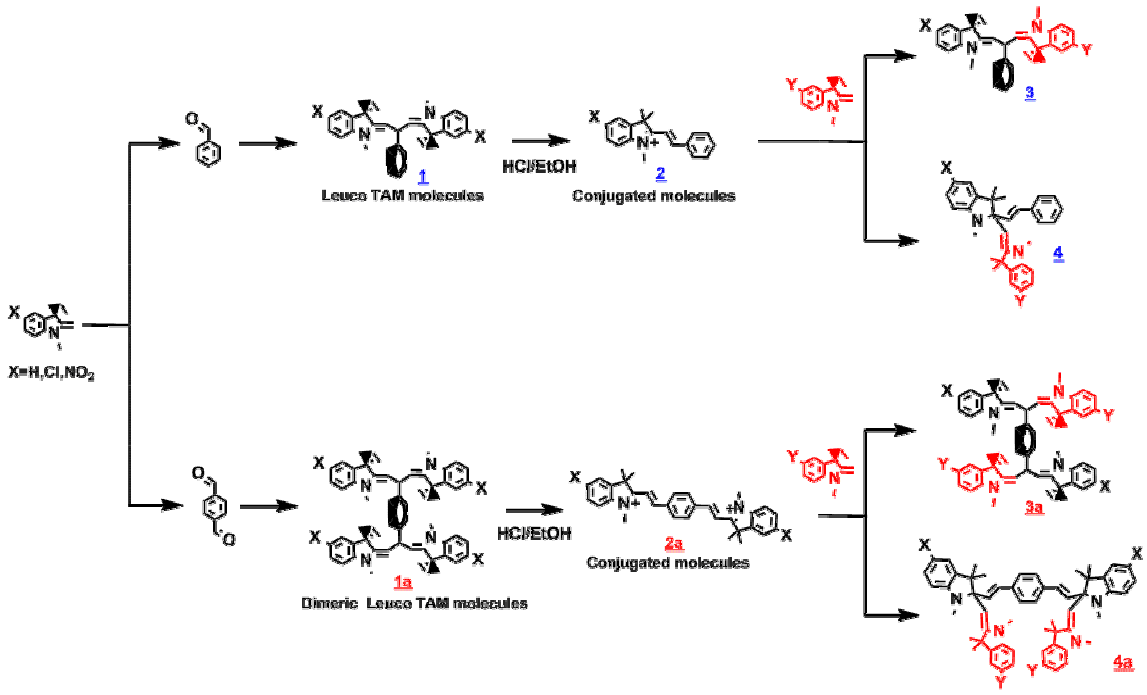
Synthesis and Spectroscopic Characterization of Asymmetric Mono- and Dimeric LTAM Derivatives

김도경, 금삼록

고려대 소재화학과

Department of Advanced Material Chemistry, Korea University, Sejong Campus 339-700, South KoreaNovel hetaryl LTAM molecules, (2Z, 2E)-2,2-(2-phenyl- propane-1,3-diylidene)bis(1,3,3-trimethylindoline) 1 and dimeric-LTAM molecules, 1-((1E,3Z)-1,3-bis(1,3,3-trimethylindolin-2-ylidene)propan-2-yl)-4-((1Z,3E)-1,3-bis(1,3,3-trimethylindolin-2-ylidene)propan-2-yl) benzene derivatives 1a were prepared from the reaction of excess 5-substituted Fischer base (FB) with benzaldehyde or terephthaldicarboxaldehyde. Acidification of the prepared LTAM dyes and dimeric-LTAM dyes can yield highly conjugated dye molecules 2 and 2a, respectively. Asymmetrical LTAM molecules 3 and dimeric-LTAM molecules 3a were prepared from the reaction of 5-substituted Fischer base (FB) with conjugated dye molecules 2 and 2a, respectively. The prepared molecules were characterized by ^{1}H, ^{13}C-NMR, UV-Vis, X-ray, EI-mass spectroscopy.



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Synthesis of Silole-Spaced Triarylmaine Derivatives

강동진, 김보라, *강영진, 이필호

*강원대 화학과 *강원대 과학교육과*

The conversion of solar energy is one of the important technologies that can replace fossil fuels in the generation of mass energy. However, the high cost of solar panels made from traditional inorganic semiconductors imposes a restriction on their mass usage. Dye-sensitized solar cells (DSSCs) is a relatively new class of low-cost solar cell. In despite of several disadvantages, DSSCs are currently undergoing rapid development to obtain robust, efficient, and cheap devices that are suitable for practical use. Recently, we have synthesized triarylamine derivatives that contain dithienosilole moiety for use in DSSCs. The synthesis of these compounds was accomplished by Stile cross-coupling reaction of triarylamine with dithienosilole in good yields.

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Synthesis of Pyrrole Derivatives from Reactions of Propargyl Acetates with Indium Tri(organothiolate)

엄다한, 이재영, 이필호

강원대 화학과

The sulfide group is a key motif in chemistry and biology. Because of the characteristic features of C-S bond as functions of biological, pharmaceutical, and material sciences, transition metal, such as Pd, Ni, Cu, Co, Rh, and Pt catalyzed C-S bond formations have received much attentions and grown up by means of the development of new catalytic systems and appropriate reagents. Recently, we reported novel and efficient Pd-catalyzed C-C cross-coupling reactions using allylindiums, allenylindiums, tri(organo)indiums, and tetra(organo)indates on the basis of the intriguing chemical properties of indium metal. However, C-S cross-coupling reactions using organoindium reagents have not been reported despite one of the principal methods forming C-heteroatom bonds. These results have led us to investigate the participation of organoindium reagents in C-S cross-coupling reactions. We report that indium tri(organothiolate) are effective nucleophilic coupling partners in Pd-catalyzed C-S cross-coupling reactions with a variety of electrophiles to produce functionalized sulfides in excellent yields. In this poster, we reported efficient synthetic method of multi-substituted pyrrole derivatives containing sulfur.

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Preparation of 1,4-Dihydronaphthalene Derivatives Catalyzed by Platinum

모준태, 서석진, 이필호

강원대 화학과

Development of an efficient cyclization method is very important for the biological and pharmaceutical applications. During the studies on the addition of allenoate to aryl substrates, we found an interesting intramolecular cyclization reaction. So, we have prepared various allenoates and their cyclization was achieved with platinum. Various type of allenoates applied to the preparation of dihydronapthalene derivatives with this catalytic system. These processes are not only efficiency but also many advantages.

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Studies on the synthesis of pyridin-2(1H)-one, pyrimidine-2,4(1H,3H)-dione and 1,2,4-triazine-3,5(2H,4H)-dione derivatives

김상혁, 손익환, 이필호

강원대 화학과

Pyridin-2(1H)-one, pyrimidine-2,4(1H,3H)-dione and 1,2,4-triazine-3,5(2H,4H)-dione derivatives is generally to gonadotropin-releasing hormone (GnRH) receptor antagonists, and to methods of treating disorders by administration of such antagonists to a warm-blooded animal in need thereof. 2,6-Difluorobenzyl acetone or benzyl acetone were treated with PPA and acetoacetamide. These resulting compound were added to bromine followed by Mitsnobu reactant and Suzuki cross-coupling reaction to give the pyrimidine-2,4(1H,3H)-dione derivatives. 1,2,4-Triazine-3,5(2H,4H)-dione derivative were obtained from reaction of 6-bromo-1,2,4-triazine-3,5(2H,4H)-dione with BSA and 2-fluoro-6-(trifluoromethyl)benzyl bromide followed by Mitsnobu reactant.

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Synthesis of 2-phenylsulfonyl cyclopropanecarboxamide derivative.

김상혁, 이상규, 이필호

강원대 화학과

2-phenylsulfonyl cyclopropanecarboxamide derivative is a representative of the sulfonamide series while as its central chemical feature. The synthesis of 2-phenylsulfonyl cyclopropanecarboxamide began with reduction of the commercially available cyclopropyl ester compound with sodium borohydride in a mixed (DME/MeOH) solvent system to give alcohol compound in good yield. Alcohol compound was then converted to its tosylate compound by treatment with p-TsCl and triethylamine in dichloromethane. The crude tosylate compound was directly converted to amine compound by treatment with one equivalent of (R)-2-methylpiperazine in acetonitrile at 70 oC, and the resulting amine was then acylated with 4-acetylbenzenesulfonyl chloride to give N,N-disubstituted piperazine 7 compound in 36% overall yield from alcohol compound (three steps). Ketone compound was converted into a 1:1 diastereomeric mixture of trifluoromethylcarbinols compound in excellent yield by treatment with TMSCF3 and TBAF in THF. Resolution of the resulting diastereoisomers was accomplished by use of a carbamate chiral auxiliary. Formation of the mixed carbonate resulting from treatment of trifluoromethylcarbinols compound with 4-nitrophenyl chloroformate and DMAP was followed by displacement of the nitrophenylphenol with commercially available (S)-(+)-2-amino-1-butanol in a single pot. The resulting mixture of diastereoisomers was separated via flash chromatography to give the pure desired diastereoisomer compound in 35% yield from trifluoromethylcarbinols compound. Treatment of diastereoisomer compound with KOH in tert-butanol at 90 oC gave 2-phenylsulfonyl cyclopropanecarboxamide derivative in good yield via hydrolysis of the nitrile to the primary amide with concomitant hydrolysis of the carbamate to the desired trifluoromethylcarbinol.

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Efficient Synthesis of vinyl allene and its application to carbocycles

최수빈, 염혜영, 이필호

강원대 화학과

Because allene is a very interesting compound having a hybrid character of C-C double and triple bond, vinyl allenes have been recognized as versatile building blocks in organic synthesis. In particular, vinyl allenes take part in not only the Diels-Alder reaction as the 1,3-diene moiety but also transition metal-catalyzed organic reactions, affording efficient synthetic methods for complex ring compounds. However, because it is not easy to effectively prepare a variety of vinyl allenes, its application to organic reactions has been limited despite the potential of vinyl allenes in organic synthesis. Although vinyl allenes were used in the Diels-Alder reactions, development of synthetic method of cyclic compounds having exo-methylene group is still required due to its utility in synthesis of natural products with biological activities. Recently, we have demonstrated that cyclic compounds having exo-methylene group were selectively produced through the Diels-Alder reaction of vinyl allene with various dienophile in good to excellent yields.

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Modified Fluorescent Nucleoside-Based Approach for Characterizing Conformational Changes of RNA Adenosine Bulges

정현석, *김병현

*포항공과대 시스템생명공학부 *포항공과대 화학과*

RNA bulges are well known dynamic structures and spotlighting targets in RNA structural research. We have investigated various factors affecting RNA bulge conformations by fluorophore labeling at RNA bulge sites and direct fluorescence spectroscopy. Several cations, various RNA structures around RNA bulges and flanking bases adjacent to RNA bulge bases determine the RNA bulge conformations. The measured fluorescent intensities based on fluorescent quenching between fluorophores and adjacent RNA bases at RNA bulge sites indicated that the flanking bases adjacent to RNA bulge bases induce conformational changes of RNA bulges. This simple and effective method of fluorophore labeling method at RNA bulges can characterize the properties of RNA bulges and promote various applications for probing specific RNA sites conformations.

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New Synthetic Method of Coumarin Derivatives

박상준, 이도형, 이필호

강원대 화학과

Coumarin derivatives exist widely in nature, especially in plants and many of them show a wide range of biological activities. Also, they are used as anticoagulants and additives in food and cosmetics and in the preparation of insecticides, optical brighteners and dispersed fluorescent and laser dyes. These properties have made coumarins into interesting targets for organic chemists. Coumarin have been synthesized by several routes including Pechmann, Perkin, Knoevenagel, Reformatsky and Wittig reactions and by flash vacuum pyrolysis. The Pechmann reaction is the most widely used method, as the reaction involves the condensation of phenols and β-ketoesters in the presence of a variety of acidic condensing agents. The use of various reagents such as H2SO4, FeCl3, ZnCl2, AlCl3 and HCl are all well documented in the literature. In this poster, we report new synthetic method of coumarin derivatives.

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Pd-Catalyzed Cross-Coupling Reaction of Aryl Iodide with Tri(ethoxycarbonylethynyl)indium

박영철, 박성국, 이필호

강원대 화학과

Transition metal-catalyzed cross-coupling reactions of organometallic reagents with electrophillic coupling partners represent one of powerful methods to generate C-C bonds. Among these, a reaction using an organoindium reagent has emerged as a favorite due to its reactivity, efficiency, versatility, and low toxicity. Recently, we have developed an efficient Pd-catalyed cross-coupling reaction of electrophilic coupling partners with tetra(organo)indates for C-C bond formation. In this reaction, in situ-generated tetra(organo)indate complexes from the reaction of indium trichloride with organometallic reagents are efficient nucleophilies in Pd-catalyzed cross-coupling reaction. Tetra(organo)indates possessing alkynyl groups effectively transferred the organic groups attached to the indium with high atom efficiency to a variety of electrophiles.

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Effective synthesis of Retinoic acid derivatives

박선영, *구상호

*명지대 나노공학과 *명지대 화학과*

Retinoic acid is a nutrient that body needs in small amounts to function and stay healthy. We developed effective and practical method for preparing retinoic acid, 13-cis-retinoic acid, retinoic acid derivatives by using C_{15}-monosulfone and various C_5-units compound, that is prepared through allylic halogenation. According to the study, retinoic acid derivatives are effectively prepared, via coupling of carbanion that is obtained from deprotonation of the C_{15}-monosulfone compound by base, with C_5-units respectively followed by dehydrosulfonation reaction.

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A Novel Process of Free Radical Cyclization

LIZHILONG, *구상호

*명지대 나노공학과 *명지대 화학과*

It is utmost important to develop biochemical and chemical methods of synthesizing cyclic structures due to their prevalence in the biologically important natural products. The controlled cyclization strategy can be diversely applied to the syntheses of cyclic natural products.We progress the research to efficiently control the mode of cascade cyclization of isoprenoid chain molecules, which can be used in the synthesis of various natural products. This method utilizes oxidative free radical cyclization of β-keto ester with Mn(OAc)3•2H2O to form the bicyclic products. We found a novel cyclization reaction, in which oxygen radical was involved to give a bicyclic compound in a highly stereoselective manner. The mechanism was already proposed based on the isolated reaction intermediates with different substrates under various reaction conditions. It is expected that the new radical cyclization can be more efficiently used in the synthesis of various kinds of natural products.

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Efficient synthetic method of various carotenoid as the nano wire

김형준, *구상호

*명지대 나노공학과 *명지대 화학과*

The carotenoids are an important class of organic molecules with delocalized π-electrons. We have perfectly demonstrated the efficient syntheses of natural carotenoids, which can be extended to the synthesis of unnatural carotenoid wires. The unnatural carotenoids can be disconnected into two parts, the allylic sulfone containing aromatic substituents and dialdehyde, for the systematic construction. These two subunits can be disconneted for the synthesis of unnatural carotenoids by the process of the following reactions: coupling, protection of the resulting alcohols, and the double elimination reactions. 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.

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A Study on Efficient and Selective Removal for Alcohols

Liang Su, 구상호

명지대 화학과

It is very interesting to activate the compounds that have more than one alcohol groups, especially selectively activate one alcohol group over the others as it is not easy to control. We have developed our method for selective removal of the allylic alcohol in the presence of non-activated alcohol. The selective reduction process of allylic alcohols was accomplished by the formation of 1-alkoxyallyl ethers and Pd-catalyzed Super Hydride reduction sequence. By applying this unique selective reduction process, we have been able to develop a new method of total synthesis of Lavandulol, which is an important additive in the perfume industry. More applications and details will be shown during the presentation.

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Synthesis of diversely-substituted allylic sulfone for the unnatural Carotenoids

임보람, *구상호

*명지대 나노공학과 *명지대 화학과*

The unnatural carotenoids have stability compared with natural carotenoid.The unnatural carotenoids can be divided to 2 part, allylic sulfone(1) unit containing sulfone and Dialdehyde unit(2) of edge side. For the construction allylic sulfone(1), containing 5 Carbon unit(C-5unit) is key point material. To the position and type of substituents, we will make the diversely substituted allylic sulfone moreover various unnatural carotenoids. By the Indium addition of haloallylic sulfone(C-5 unit), we can get homoallylic alcohol. The reaction provides high stereoselectivity and absolute regioselectivity. By the oxonia-cope rearrangement of various condition of Lewis acid, homoallylic alcohol produces the allylic sulfone.

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Highly Selective and Reversible Peptide Sensor for Monitoring in 100% aqueous solutions

김정민, Lohani Chuda Raj, 이건형

인하대 화학과

Recently, peptide probe sensors which work in aqueous solution have increased attention of the scientific community. A new fluorescent peptide probe for the detection of Ag+ was synthesized in SPPS with Fmoc chemistry. CP1-i was synthesized by inter-disulfide bond formation of Dansyl-CPGH-NH2 using Oxidized DTT. The peptide sensor has a good solubility in aqueous buffer system; thus we investigated the fluorescence response to various metal ions in physiological buffer solution without any co-solvent. Among the 14 metal ions, CP1-i shows turn on response to Ag+ and turn-off response to Cu+ and Cu2+ in 10 mM HEPES buffer solution (pH 7.4). Further experiments suggested the peptide sensors shows distinct advantages for sensing Ag(I) ions in 100 % aqueous solution such as a fast, reversible, hypersensitive, and turn-on responses.

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Pyrene based fluorescent chemosensors

정용숙, *윤주영

*이화여대 바이오융합과 *이화여대 화학과*

The synthesis of fluorescent chemosensors has been an important role in recent few years due to the simplicity and high detection limit. Pyrene containing molecular systems which show switching the monomer/excimer emissions demonstrate highly selective fluorescent changes depending on the various chemical environment (matal ions, anions, pH). Few examples of pyrene derivatives and their fluorescence changes by external inputs will be proposed.

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New Colorimetric and Fluorescent Sensors based on the PDAs

이경미, *김성진, **이진용, *윤주영

*이화여대 바이오.융합대학원 *이화여대 화학과 **성균관대 화학과*

Conjugated polydiacetylenes (PDAs), have alternating ene-yne backbone structures, can be made by the UV irradiation of self-assembled diacetylene (DA) supermolecules. In addition, the distinctive characteristics of PDAs, which arise a blue-to-red color shift under the stimulus environment, enables it to be employed as PDA-based chemosensors. Developing an convenient anionic surfactant sensor in water is very important for the detergent industry on account of environmental pollutant. A new PDA bearing imidazolium groups display large fluorescence enhancement and colorimetric change in presence of anionic surfactants.

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Imidazolium based receptors for anions.

송나리, *윤주영

*이화여대 바이오융합과학대학원 *이화여대 화학과*

The design and synthesis of anion selective receptors or sensors is a topic of great current interest. Among the various types of these receptors, imidazolium based receptors have been actively investigated and utilized for the recognition of anions because imidazolium group can make a strong interaction with anions by virtue of formation of strong $[C\text{-}H]^{+} \bullet\bullet\bullet X^{-}$ type ionic hydrogen bonding. This novel type of charged hydrogen bonding is very different and intriguing in comparison with many other conventional hydrogen bonds. In the present study, we have synthesized several receptors bearing imidazolium and naphthoimidazolium group including couple of cyclophane type receptors. The synthesis of these receptors as well as their binding studies will be presented.

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An hypersensitive water-soluble fluorescent probe for Hg(Ⅱ) ions based on L-methionine

양미화, 이건형

인하대 화학과

A hypersensitive water-soluble fluorescent probe, dansyl-L-methionine was synthesized in solid phase synthesis. This fluorescent probe displayed remarkable advantages including turn-on fluorescence properties upon Hg(Ⅱ) addition, rapid and specific response to Hg(Ⅱ) in 100% aqueous solution. The sensor that has a simple structure satisfies for monitoring the maximum allowable level (2 ppb, 10 nM) of Hg(II) in drinking water demanded by EPA via a turn-on response in a neutral buffer solution.

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Synthesis of Pyrene –based Peptide sensors for Metal ions

kachi reddy kishore kumar reddy, 이건형

인하대 화학과

Due to the widespread applications, transition and heavy metal ions play an important role in many biological and environmental processes. The development of molecular sensors is an important goal of broad consequence, ranging from a variety of natural and environmental contaminations of heavy and transition metal (HTM) ions causes serious problems for human health and ecology. Fluoroionophore chemosensors are becoming increasingly popular due to their easy use in solution as well as their high sensitivity to and selectivity for trace analytes.Based on above importances we choose different pyrene analogues (pyrene carboxilic acid, pyrene sulphonyl chloride and N,N-dimethyl pyrene sulphonyl chloride) as a fluorphore and synthesised pyrene-peptides. Their selectivity, sensitivity and reversibility properties were studied for metal ions in 10 mM HEPES buffer pH 7.4.

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Microwave-assisted amide bond synthesis by conjugation of 6-Monodeoxy 6-amino-Cyclodextrin with C-term peptides

Lohani Chuda Raj, 김정민, 이건형

인하대 화학과

A new procedure was developed for reducing the reaction time and improving the yield of amide synthesis reaction between C-term peptide and 6-Monodeoxy 6-amino b- Cyclodextrin in solution phase by utilizing microwave irradiation. We selected a Glycine as a control aminoacid and optimized the microwave-assisted amide reaction (Fmoc-Gly-CO-NH-bCD). For this, microwave-assisted amide reactions with different reaction time, temperature, and solvents were performed using 1,3-diisopropylcarbodiimide (DIC) as the coupling reagent. We synthesized several peptides containing an amide bond by using the optimized microwave irradiation method. The purity and yield of the peptides synthesized in this way were better than those obtained without microwave irradiation. Furthermore, we applied this methodology for synthesizing long chain peptides (6- and 12-mer) corresponding to the α helical peptide. The microwave-assisted amide reaction afforded the target peptides with high yield (80%) and purity within 10 min, whereas the reaction without microwave irradiation afforded the target compound with poor yield (30%) and long period (24 hr).

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Synergic Effect of Pd(II) and Acid Catalysts on Tandem Annulation Reaction for the Regioselective Synthesis of Ring-Fused Quinolines

옥수경, *윤소원, 강용철

*부경대 화학과 *한양대 화학과*

Recently, we have developed tandem cyclization reaction of o-alkynylanilines and aldehydes to afford ring-fused quinolines. The combination of Pd(II) and protic acid catalysts exhibited synergistic effect to improve the efficiency of this tandem cyclization. Rational design of catalytic system and exquisite tune of catalysts and reaction conditions could modulate the reaction propensity and reaction pathway for the regioselective synthesis of quinoline derivatives. Although more detailed investigations are needed to clarify the mechanism for the present reaction, it is likely that this tandem reaction proceeds via a reaction pathway involving alkyne activation by coordination to Pd(II) as well as imine activation by acid alone or by acid and Pd(II) together. This regioselective one-pot reaction offers considerable advantages with regard to simplicity and high efficiency.

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Rh(I)-Catalyzed Tandem Conjugate Addition and Cyclization Reactions for the Synthesis of Dihydroquinolinones, Dihydrocoumarins, and Pyrrolidinones

박자옥, *윤소원, 강용철

*부경대 화학과 *한양대 화학과*

Recently, we have developed a new Rh-catalyzed tandem conjugate addition and cyclization reaction to afford 4-aryl-3,4-dihydro-2(1H)-quinolinones, 4-aryl-3,4-dihydrocoumarins, and 4-arylpyrrolidin-2-ones. In this process only arylboroxines were effective among a variety of organoboron reagents. This process represents an mild and facile construction of a variety of heterocycles, which are important motifs in both naturally occurring and biologically active compounds.

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발표종류: 포스터, 발표일시: 금 10:30~12:30

Synthesis of small molecule library using solid phase combinatorial chemistry

김주리, 신인재

연세대 화학과

Small molecules can perturb the function of their targets and are useful tools to dissect dynamic cellular processes. Herein, the solid phase synthesis of the imidazole library is described. The imidazole library would be powerful tools for the elucidation of protein-small molecule interactions and the screening of the drug candidates by high-throughput assays based on cultured cells and chemical chip. Various imidazole derivatives show a broad range of bioactivities, such as antineoplastic, immunosuppressive, and anti-inflammatory activities. Thus we synthesized an imidazole library with diverse substituents at the positions of 1, 2, 4, or 5 on a solid support to identify active compounds inducing interesting differentiation in cells, such neurogenesis.

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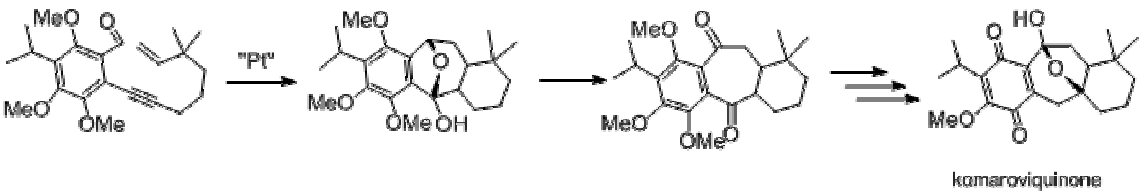
Synthesis of komaroviquinone by Pt-catalyzed intramolecular cyclization

오창호, PIAOLANHUA

한양대 화학과

The nature product-Komaroviquinone is a kind of tricyclic compound which shows strong vitro trypanocidal activity against epimastigotes of Trypanosoma cruzi, the causative agent of Chagas' disease in Central and South America. The total syntheses of several related diterpenes, which incorporate a functionalized 6-7-6 fused tricyclic Framework have appeared in the literature and involved generation of the basic skeleton mainly through acid-catalyzed cyclialkylation reactions. Our team reported Rh-catalyzed [3+2]-cyclization and gold catalyzed [3+2]-cycloisomerization of o-akynylbenzaldehydes with unsaturated bond and synthesized faveline Methyl Ether by using Pt-catalyst. Encouraged by this expected result, we planned to synthesize komaroviquinone and performed it by Pt-catalyzed intramolecular cyclization reaction. The general scheme is shown as follows.



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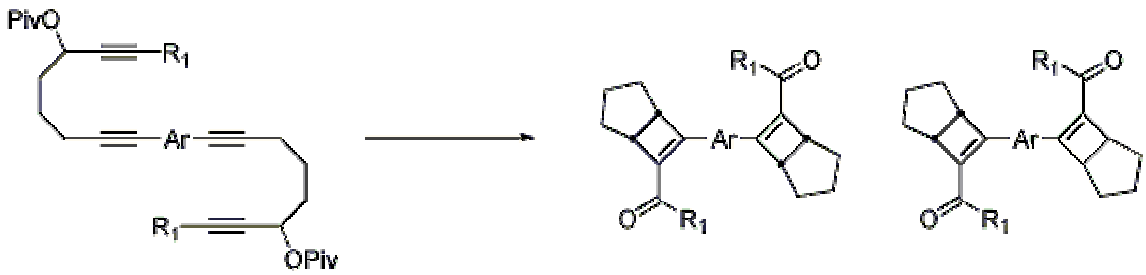
발표종류: 포스터, 발표일시: 금 10:30~12:30

Gold catalyzed intramolecular [2+2] double cycloaddition of bis-alkyne propargylic pivaloates to bis bicyclo compounds.

오창호, 이규환

한양대 화학과

Transition metal catalyzed cycloisomerizations of polyunsaturated systems are atom economic and environmentally benign synthetic methods to provide efficient access to a variety of structural motifs in many natural products and useful building blocks in synthetic chemistry. Due to the excellent alkynophilicity of gold, particular attention has been paid to gold based alkyne activatie activation as an attractive strategy for developing new and efficient catalytic cyclizations. We have discovered a highly convenient gold catalyzed cyclization of bis-alkyne propagylic pivaloates leading to bis bicyclic compounds, that could provide an easy access to valuable building blocks for conjugated polycyclic compounds.



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A one step, acid mediated method for modification of glass surfaces with N-hydroxysuccinimide esters and its application

배재영, 박성진, 신인재

연세대 화학과

Microarray technologies have received considerable attention owing to the fact that they serve as effective tools for high-throughput analysis of boimolecular interactions and the identification of bioactive substances that bind to biomolecules. Most of the current metho d used to construct microarrays rely on the immobilization of substances on properly derivatized surfaces. Among various functional groups used for this purpose, the N-hydroxysuccinimide (NHS) ester group has been largely employed since it can be readily reacted with amine or hydrazide functionalities in substances of interest. However, the NHS ester group is usually introduced onto the surface of a glass slide by employing inconvenient and time consuming multi-step processes. In recent studies, It was developed an efficient, single step method for derivatization of glass surfaces with NHS ester groups that takes advantage of an acid-mediated reaction of NHS ester functionalized dimethallysilanes with silanols on the glass surface. Conditions for the surface modification procedure that utilize TfOH rather than Sc(OTf)3 were found to be superior. Protein and RNA-binding experiments show that glass surfaces Modified by employing this method are suitable for efficient immobilization of various substances that are appended by amine, hydrazide and alcohol functionalities. The microarrays, generated in this way, are applicable to procedures for rapid analysis of protein-protein, protein-glycan, protein-small molecule and peptide and peptide-RNA interactions, as well as for profiling enzyme activities. The newly developed acid-mediated, glass surface modification method should be generally applicable to the preparation of various functional group-modified surfaces.

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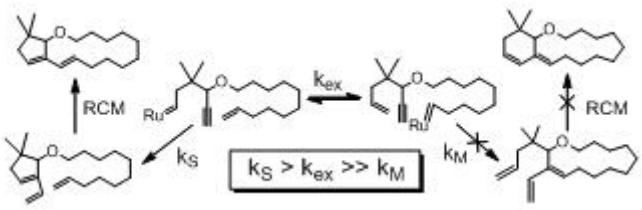
Synthesis of Small and Large Fused Bicyclic Compounds by Tandem Dienyne Ring Closing Metathesis

박현, 최태림

서울대 화학부

Synthesis of fused bicyclic compounds comprising small and large membered ring by tandem enyne ring closing metathesis was carried out successfully. While tandem enyne ring closing metathesis reaction suffers due to the catalyst non-selectively reacting with one of two terminal alkenes to give two different products with different ring size, rate of cyclization of small sized ring is far greater than that of macrocyclic ring compounds and gives single isomer. We successfully performed this reaction with 14 different kinds of substrates, where small ring size varies from 5 to 7 and large ring size from 14 to 17. Latter formed alkene group in macrocycle gives pure *E* stereoselectivity with some exceptions. Details will be discussed in poster session.



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Dipyrenylcalix[4]arene Chemosensor for the Detection of Trinitroaromatic Explosives

이영훈, 김종승

고려대 화학과

A novel approach based on fluorescence quenching with dipyrene-functionalized calix[4]arene is presented for the detection of nitrated aromatics. Trinitroaromatics such as TNT and TNB acts as more effective quenchers than singly or doubly nitrated aromatic compounds. We reported the molecular structure of L·TNT complex by X-ray crystallography to prove the binding circumstance between electron donor and acceptor, exhibiting the formation of supramolecular crystalline polymeric structure not only by intermolecular interaction with two neighboring pyrene substituents and aromatic counterpart of TNT in the distance of around 3.2 ~ 3.6 Å but also by intra- and intermolecular hydrogen bonds among amides. We also observed the color changes of L·TNT and L·TNB complexes from colorless to a reddish orange under more or less the high concentration by charge transfer arising from complementary π-π complexation between pyrene and trinitroaromatics.

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Synthesis and Characterization of Shape-Selective Porphyrin Chemosensors bearing Polyhedral Oligomeric Silsesquioxanes

정은희, *이창희

*강릉대 화학과 *강원대 화학과*

본 연구는 기존의 포르피린 콘쥬게이션의 변화를 주어 다양한 음이온 감지에 따른 색 변화 방법과는 차별화된 방법으로, 입체 장애가 큰 Polyhedral Oligomeric Silsesquioxanes (POSS) 작용기를 포르피린에 도입하여 유사한 크기의 음이온 감지 능력 향상을 꾀하는 데 있다. POSS 를 포르피린에 도입함에 있어 포르피린 벤젠고리의 오쏘, 메타, 파라 등 다양한 위치에 도입하여 이로 인한 입체장애의 차이점으로 인해 음이온 감지 시 나타나는 색깔의 변화를 탐색하고자 이들을 합성하였고, 이들의 분광학적 특징을 NMR, UV, IR 을 통해 살펴보았다.

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New Multi-BODIPY Molecules and Their Host-Guest Complex Formation with Cucurbit[*n*]uril

신지영, *N. Selvapalam, **김기문

*포항공과대 첨단재료과학부 *포항공과대 화학과 **포항공과대 화학과 첨단재료과학부*

Boron dipyrromethene (BODIPY) dyes attract considerable attention owing to their remarkable photochemical properties such as high molar extinction coefficients, high fluorescence quantum yields, long excited singlet-state lifetimes and thermal/photochemical stabilities. Numerous applications of BODIPY dyes such as biological labeling, fluorescent sensors, luminescence devices, synthetic light harvesters, photonic devices, and drug delivery templates have been reported. In an effort to explore new applications of BODIPY dyes, we have synthesized several multi-BODIPY molecules including BODIPY-porphyrin hybrids. In addition, we studied the host-guest complex formation of the BODIPY dyes with cucurbit[*n*]uril (CB[*n*]), a family of host molecules with a hydrophobic cavity. Photochemical properties of the BODIPY dyes and their complexes with CB[*n*] will be presented.

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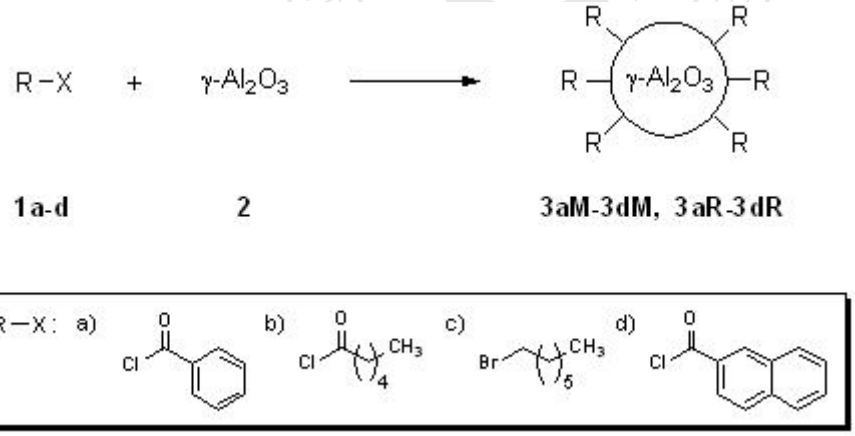
Functionalization of γ-Alumina with Organic Ligands; Luminescence Hybrid Material

장석명

창원대 화학과

The functionalization of γ-Alumina with organic compounds is developed to prepare the organic-inorganic hybrid luminescent material. In this paper 1]we will discuss the convinient reaction method which is microwave irradiation or refluxing. 2]The characterization of organic-inorganic hybrid luminescent material will be discussed.



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Synthesis of (Z)-2-alkylidene-4-(1-phenylethyl)-3,4-dihydro-2H-benzo[b][1,4]thiazine-3(4H)-thiones

이은영, 김신형, 신동수

창원대 화학과

(Z)-2-Alkylidene-4-(1-phenylethyl)-3,4-dihydro-2H-benzo[b][1,4]thiazine-3(4H)-thiones were prepared by the reaction of N-substituted 4H-benzo[1,4]thiazine-3-thione with the appropriate aldehydes. N-Substituted 4H-benzo[1,4]thiazine-3-thione was prepared via Smiles rearrangement using microwave irradiation by one-pot synthesis, followed by the reaction with P2S5 in presence of NaHCO3.

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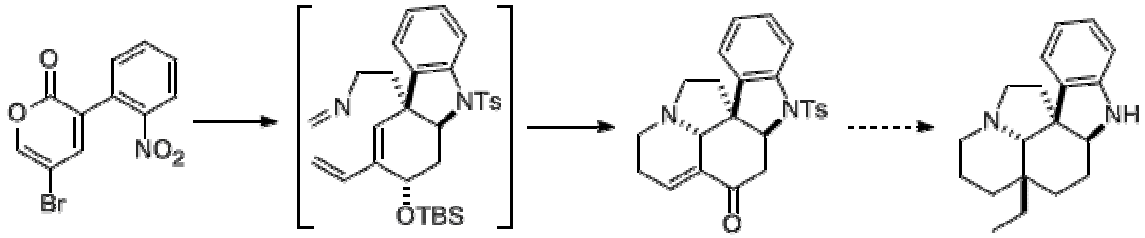
Hetero-IMDA approach toward the aspidosperma alkaloids from 3,5-dibromo-2-pyrone

조천규, 권진

한양대 화학과

Aspidosperma alkaloid family comprises one of the largest groups of indole alkaloids with more than 250 members. Structurally, aspidosperma alkaloids share a common characteristic pentacyclic ABCDE framework where the central C-ring possesses all stereocenters and significant functional groups. Because of a wide range of intriguing biological activities portrayed by many of the members, a considerable research interest has been devoted in their synthesis, leading to the development of many efficient and elegant synthetic methods and routes Further envisaged was the Diels-Alder adduct of 3-aryl-2-pyrone with vinyl ether would provide all the necessary funtional groups with correct orientation required for the synthesis of aspidosperma alkaloids. Herein, we report the preliminary acccount of our 2-pyrone strategy to the synthesis of the key framework of aspidosperma alkaloids.



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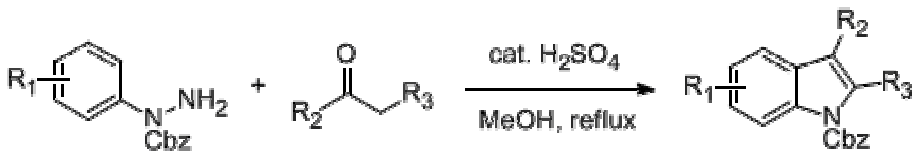
Aryl hydrazide beyond as surrogate of aryl hydrazine in the Fischer indolization: the synthesis of N-Cbz-indoles, N-Cbz-carbazoles and N,N'-bis-Cbz-pyrrolo[2,3-f]indoles

조천규, 박인걸

한양대 화학과

The indole nucleus is arguably the most privileged molecular scaffold in nature. A wide variety of important biological activities featured by a plethora of indole-based natural products have driven them to be highly attractive targets for synthesis over the years. A number of elegant synthetic methods and strategies, most notably those based on the Pd-catalyzed C-N bonding formation, have been developed and successfully applied for the synthesis of indoles and related products. The Fischer indole synthesis, reported over 100 years ago, still remains of considerable value, although somewhat compromised by the poor availability of the starting aryl hydrazines. In our previous report, we have demonstrated that aryl hydrazides 1 are effective surrogates of aryl hydrazines in the Fischer indolization reaction. Recently, we found that aryl hydrazides bearing more acid stable N-Cbz group(s) can undergo the Fischer indolization reactions to the corresponding indoles while the N-Cbz group(s) remained intact.



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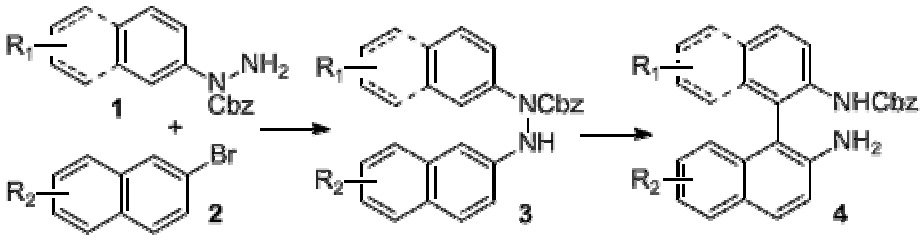
Synthesis of mono-N-Cbz-1,1'-diaryl-2,2'-diamines via acid-catalyzed [3,3]-sigmatropic rearrangement of diaryl hydrazide

조천규, 서성은

한양대 화학과

Axially chiral biaryls are important structural scaffolds which have permitted advent of various asymmetric chiral ligand systems proven to be effective in a wide variety of enantioselective transformations including Diels-Alder, Mukaiyama aldol and hydrogenation reactions. The biaryl cores are primarily synthesized through the Cu(II), Fe(III), Mn(III) or V(IV)/O2 mediated oxidative couplings of aryl alcohols. The resulting biaryl diols serve as platforms for other biaryl ligands including the famous BINAP and its derivatives. Much less explored than BINAP type ligands, the nitrogen analogue, BINAM and its N-substituted analogs have recently emerged as new powerful chiral ligands and organocatalysts. However, further exploitation is much hampered by the lack of general synthetic methods. We found that diaryl hydrazides 3 bearing an acid stable N-Cbz group can undergo the acid-catalyzed [3,3]-sigmatropic rearrangement reaction to afford mono-N-Cbz-2,2'-diamino-1,1'-biaryl 4 in good overall yields.



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1,2,3-Triazolium-based ionic liquids as a novel class of phase transfer catalyst

이자영, *이병세, 지대윤

*서강대 화학과 *(주)퓨처켐 표지화학연구소*

Imidazolium-based ionic liquids (ILs) play a role in heterogeneous nucleophilic substitution reaction as either reaction media or phase transfer catalyst (PTC). Development of efficient PTC is very important for ^{18}F-radiopharmaceutical research and industry. To this end, we prepared a series of 1,2,3-triazolium-based ILs in two step synthesis, copper(I)-catalyzed azide-acetylene cycloaddition (CuAAC) followed by quarternization. Two functional groups were readily tailored by CuAAC reaction of various azide and acetylene compounds. Some ILs have one or two tertiary alcohol functional groups for better chemoselectivity via hydrogen bonding with fluoride ion. The newly prepared ILs were evaluated in heterogeneous nucleophilic fluorination.

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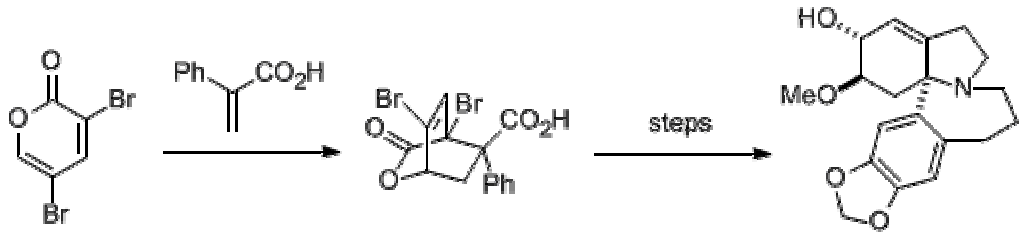
발표분야: 유기화학
발표종류: 포스터, 발표일시: 금 10:30~12:30

Progress toward total synthesis of (±)-homoerythratine

조천규, 송지영

한양대 화학과

Homoerythrina alkaloids, comprised of more than 70 members, possess an intriguing azatetracyclic skeleton. They can be grouped into two subcategories based on the structural type of D-ring; aromatic or nonaromatic. The homoerythrina alkaloids are biosynthetically related and structurally similar to the Erythrina alkaloids, except mostly in size of ring-C (azacyclohexene ring in the Erythrina alkaloids vs azacycloheptene ring in the homoerythrina alkaloids). While many of the Erythrina alkaloids proved biologically active, little is known on the pharmacological effects of the homoerythratine family alkaloids. As a part of our ongoing research program exploring the synthetic utility of 3,5-dibromo-2-pyrone and its derivatives as novel enophile synthons, we have envisaged the cycloadduct with 2-aryl acrylic acid can be readily converted into homoerythrina alkaloids. Presented herein would be our preliminary account on the total synthesis of (±)-homoerythratine



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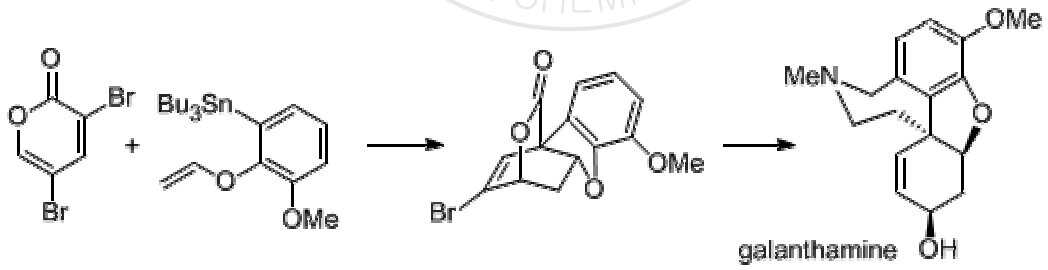
Total synthesis of (±)-galanthamine via the coupling/IMDA cascade of 3,5-dibromo-2-pyrone

조천규, 장재혁

한양대 화학과

Galanthamine has potent inhibitory activity against acetylcholinesterase(Ache) in CNS, and has been approved for the treatment of Alzheimer's patients through the enhancement of their cognitive functions. As a part of our ongoing research program on 3,5-dibromo-2-pyrone as novel enophile synthons, we have explored its potential applicability to the target-oriented synthesis with the maximum use of the resultant densely functionalized cycloadducts. We have recently achieved the total synthesis of galanthamine, using the regioselective coupling reactions of 3,5-dibromo-2-pyrone and IMDA as key steps. Presented herein is the detail on the total synthesis of galanthamine.



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발표종류: 포스터, 발표일시: 금 10:30~12:30

Fast and mild synthesis of 18F-Labeled click prosthetic groups for PET study.

이보람, *이병세, 지대윤

*서강대 화학과 *(주)퓨처켐 표지화학연구소*

Positron emission tomography has received a great attention as a clinically applicable molecular imaging tool. Of various positron emitters, F-18 is the most attractive on the basis of a proper half-life of 110 min. Unlike small synthetic molecules, a [18F]radiofluorination of biomolecule-based disease targeting substances needs a special and careful treatment during synthesis and purification. We have developed two 18F-labeled prosthetic groups, i.e., succinimidyl ester and maleimide using copper(I)-catalyzed azide-acetylene cycloaddition (CuAAC). While previous methods comprise multi-step synthesis and long preparation time, click method offered not only short synthetic steps and time, but also high radiochemical yield (RCY) and purity (RCP). Our method consists of two steps, [18F]fluorination and click ligation. [18F]Fluorination of azide precursor was completed in 10 min under heating at 120 oC, with excellent RCY. After simple silica filtration, the resulting filtrate was reacted with ethynyl succinimidyl ester or ethynyl maleimide in the presence of CuI.

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Synthesis and characterization of chlorin based anticancer drug conjugate

Gantumur Battogtokh, *안웅식

*Cancer Institute of Medical Science, The Catholic University of Korea *가톨릭대 산부인과*

Photodynamic therapy (PDT) is a promising approach to cancer treatment. PDT is based on the combination of a photosensitizing agent and light. Chlorin-based photosensitizers are considered to meet requirements for the ideal photosensitizer in PDT. They have improved efficacy and have lesser known side effects compared to porphyrin-based photosensitizers. Paclitaxel (PTX) and cis platinum are the most effective and widely used drugs for chemotherapy. Although chemotherapy is a powerful and an important modality in cancer treatment, the effectiveness of the chemotherapy is limited by systemic toxicity and side effects of agents used.For the syntheses, naturally occurring chlorin derivatives were used as starting material. It was prepared with the acidic treatment of methyl pyropheophorbide-a (MPPa) from Spirulina maxima algae according to the previously reported methods [1-2]. Then, pyropheophorbide-a (PPa) was prepared from MPPa. The paclitaxel (PTX) and PPa were conjugated through estrification reaction using DCC coupling agent in the presence of DMAP. To synthesize the chlorin-based platinum conjugate, PPa bearing free amine was primarily prepared, which was reacted by treating with potassium tetrachloroplatinate in the mixture of tetrahydrofuran and water. The structures of PTX-PPa and chlorin-based cis platinum conjugates were fully characterized by proton NMR (1D and 2D), MALDI-MS, UV-vis, ICP mass, IR and elemental analysis techniques.The conjugates can be applied as anticancer agents for PDT of tumor cell and is promising to be able to afford some synergistic effects.References: 1. Smith, K. M.; Goff, D. A.; Simpson, D. J.; J. Am. Chem. Soc. 1985, 107, 4946-4954.2. Galindev, O.; Badraa, N.; Dalantai, M.; Sengee, G.; Dorjnamjin, D.; Shim, Y. K. Photochem. Photobiol. Sci. 2008, 7, 1273-1281.

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Optical Properties and Redox Properties of Heteroaromatic Ring Compounds Containing EDOT

정연준, 김인태, 이상우

광운대 화학과

Thiophene based linear π-conjugated oligomers have their potential applications for active materials in organic electronic and photonic devices. Therefore electronically conducting poly(3,4-ethylenedioxythiophene)(PEDOT) has been regarded as an excellent material to be applied to in electronic devices, electrolytic capacitors, actuators, sensors, artificial muscles and LEDs. Herein, we synthesized EDOT based linear π-conjugated oligomers containing hetero aromatic compounds with unique electronic and opitical properties. The structure of the resulting compounds were characterized by ^{1}H NMR, ^{13}C NMR, and FT-IR. The optical property and electronic property of the resulting compounds were measured by UV-vis spectroscopy and cyclovoltammetry, respectively.

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Terpyridine Receptor-Immobilized Silica-Coated Magnetic nanoparticles As a General Binding Agent for Histidine-Tagged Proteins

조은진, *정세라

*전남대 임산생명공학부 *전남대 임산가공학과*

A new terpyridine receptor-immobilized silica-coated magnetic nanoparticles (TSMNPs) as selective magnetic probes of His-tagged proteins was synthesized and characterized by transmission electron microscopy (TEM), X-ray diffraction (XRD) analysis, FT-IR spectra, and fluorescent spectroscopy. The His-tagged protein binding capacity and purification efficiencies of the fluorescent TSMNPs is higher than the commercial Ni-NTA His-tag affinity chromatography. This simple system serves as a useful alternative to existing protocols for his-tagged protein separation and as a versatile agent for transporting and anchoring proteins.

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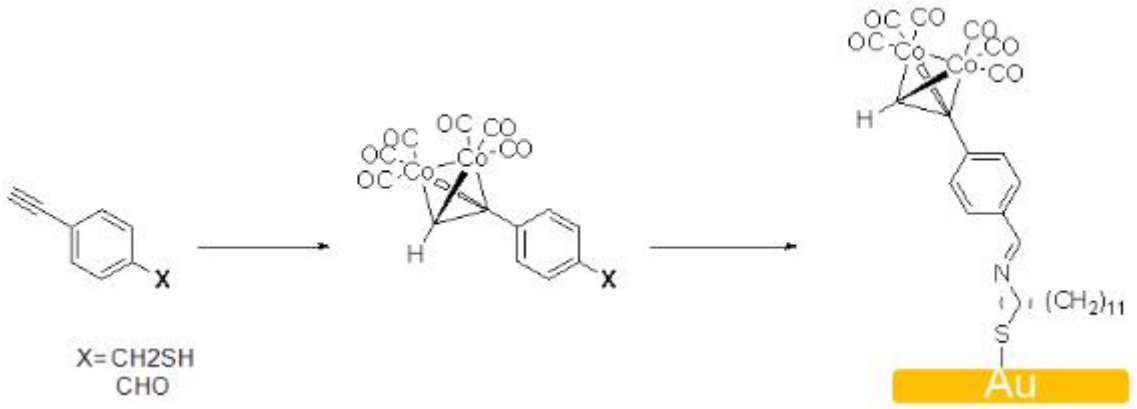
Formation of SAMs and Photolysis of Alkyne-Cobalt Complex on Gold Surface.

이영배, 황광진

홍익대 화학시스템공학과

표면에서 알카인 작용기의 고정화는 바이오 칩, 센서 등 다양한 분야에서 활용할 수 있다. 표면에서의 광반응을 이용하면 고정화된 알카인 전구체를 위치 선택적으로 개질하여 다양한 형태의 패턴 형성이 가능하다. 극자외선을 이용한 미세 패턴의 형성을 위해서는 초점심도가 작은 자기조립 분자막의 형성이 필요하다. 표면에서의 광분해반응이 가능한 알카인 전구체로서 알카인-코발트 착화합물에 관심을 가지고, 표면에서의 자기조립박막 형성과 광분해반응을 고려하여 알데히드기를 가지고 있는 알카인-코발트 착화합물과 알카인-코발트-포스핀 착화합물을 합성하였다. XPS(X-ray photoelectron spectroscopy)를 측정하여 골드 표면에 화합물의 자기조립박막이 형성하였음을 확인하였고 빛을 이용한 분해반응을 진행하였다. XPS 와 IRRAS(Infrared reflection absorption spectroscopy)를 이용하여 표면의 변화를 측정하였다.



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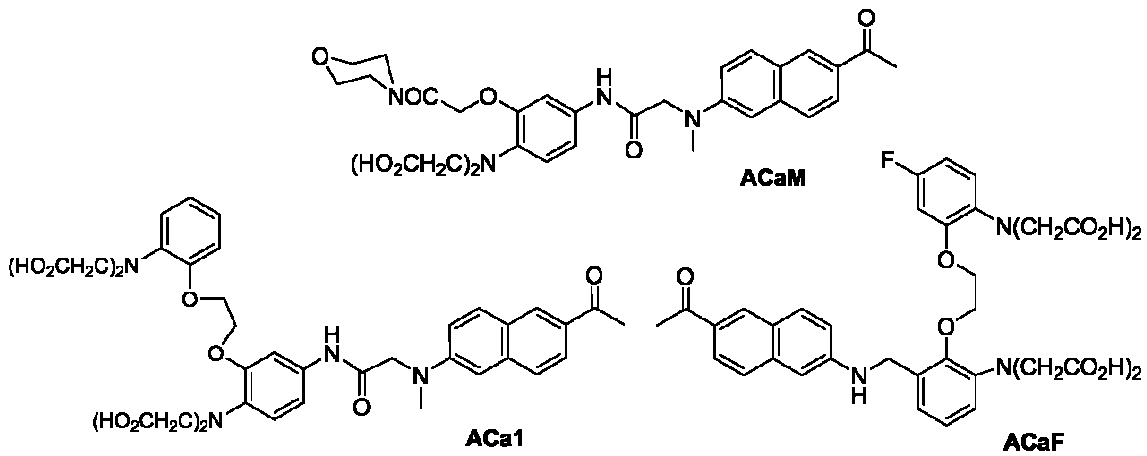
Two-Photon Probes for Long-Term Imaging of Levels of Ca^{2+} Ions

Palathurai Subramaniam Mohan, *임창수, Yu Shun Tian, *한지희, *조봉래

*Korea university *고려대 화학과*

Herein, we report an efficient two-photon probe that can visualize the calcium distribution in the live tissues. In this work, we extend our previous work and present a series of TP probe (ACa1-ACaF-ACaM) that can be excited by 780 nm photons, show 40-6-2-fold two-photon excited fluorescence enhancement (TPEF) in response to Ca^{2+}, and the dissociation constants(K_dTP) were (0.23 ± 0.02)-(0.43 ± 0.03)-(116.20 ± 0.02) μM upon complexation with Ca^{2+}. Unlike the previously available probes, these novel probes can selectively detect dynamic levels of Ca^{2+} ions in live cells and living tissues without interference from other metal ions and from the membrane-bound probes, because of their different K_d value. Moreover, these probes are capable of monitoring the calcium waves about > 100 μm depth in live tissues for long time using TPM with no artifacts of photo-bleaching.



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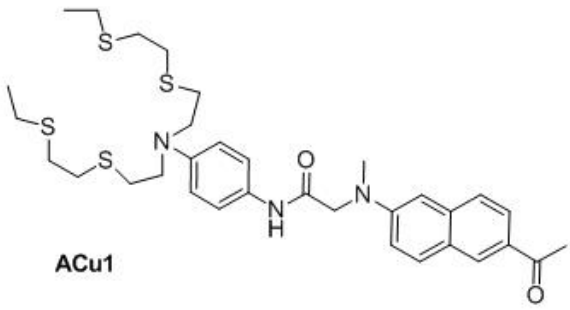
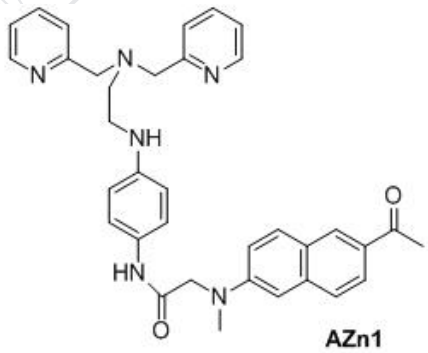
A Noble Study of Gastric and Colon Cancer by Multiphoton Laser Scanning Microscopy

임창수, *Yu Shun Tian, 강동원, 김창우, 조봉래

*고려대 화학과 *KOREA UNIVERSITY*

Several studies suggest the Cu/Zn ratio is a good indicator of the extent and prognosis in carcinoma of the gastrointestinal tract. However, there has been no attempt to visualize their distribution in cancer tissues. The aim of this study is to evaluate the utility of TPM for the diagnosis of gastric and colon cancers. For this purpose, we have developed new TP probes for Zn and Cu ions, detected the metal ions in normal and cancer cell lines, visualized their distributions in normal mucosa, adenoma, and adenocarcinoma tissues by TPM using the TP probes, and assessed their relevance to the gastric and colon cancers.





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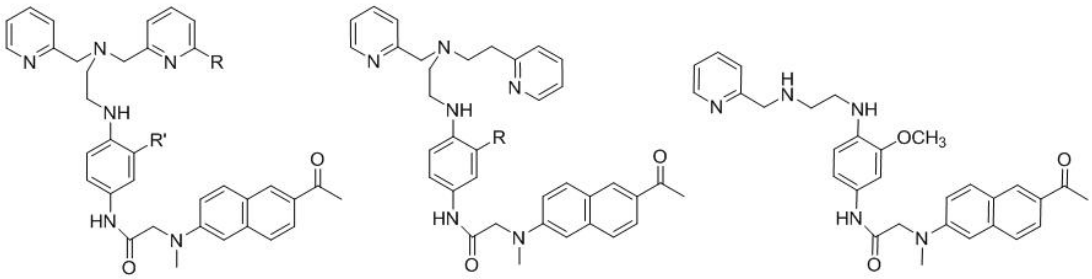
Two-Photon Zinc Selective Probes with Various Affinities for Imaging in Live Cells and Tissues

Isravel Antony Danish, *임창수, *정철, *한지희, *김창우, *황혜림, *조봉래

KOREA UNIVERSITY *고려대 화학과

We report a series of fluorescent two photon Zn^{2+} selective sensor molecules, AZNM1-AZNn with different dissociation constants, because the concentration of Zn^{2+} in biological system differs over a wide range from sub-nanomolar to millimolar. Thus prepared sensors have K_d values in the range of 10^{-9}-10^{-5} M, compared with 0.5 nM for previously reported AZn2. All the compounds were having a solubility of 3.0 μM and are not affected by the presence of other biologically important metal ions such as calcium or magnesium, they can detect Zn^{2+} within 100 ms. The bright field image of a part of fresh hippocampal slices incubated with 10 mM AZnM2, AZnE1, AZnE2, and AZnN revealed the CA1 and CA3 regions as well as the dentate gyrus (DG). The TPM images AZnM2-labeled tissue clearly revealed the Zn^{2+} distribution of the same regions at 80-170 μm depth Thus, by using a combination of sensor molecules, it was shown that a higher Zn^{2+} concentration is released in DG than in CA3 or CA1 and that we can easily visualize Zn^{2+} concentration over a wide range. We has shown that these probes are highly suitable to detect Zn^{2+} in live cells and living tissues at 100 μm depth with high resolution and without mis-targeting.



R = H, R' = H (AZn1)
R = H, R' = OMe (AZn2)
R = Me, R'= H (AZnM1)
R = Me, R' = OMe (AZnM2)

R = H (AZnE1)
R = OMe (AZnE2)

AZnN

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Au(I)-Catalyzed Intramolecular Cyclization Reactions of Alkenyl β-Keto Esters

Arun R. Jagdale, 박종협, 윤소원

한양대 화학과

β-Keto esters are one of the most widely used building blocks in organic chemistry and undergo various types of substitution reactions. Particularly, β-keto esters undergo C-C bond formation reactions in the reaction with carbon elecrophiles. However, electrophilic addition reactions of β-keto esters are rare in the literature. More interestingly, transition-metal-catalyzed nucleophilic addition reactions of β-keto esters to olefins have been well reported in which β-keto esters usually act as a nucleophile to afford cyclic compounds.Recently, we have discovered a novel synthetic method for the synthesis of indene derivatives in good yields. $Ph_3PAuCl/AgOTf$ catalyzed effectively the intramolecular addition reactions of alkenes to β-keto esters to provide a variety of substituted indenes in moderate to high yields. In addition, this catalytic system was found to be very effective for the carbonyl-ene reaction of allylic β-keto ester derivatives to afford naphthalenes in high yields.

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N-Heterocyclic Carbene-Catalyzed Oxidative Cyclization Reactions: Synthesis of Phthalides and Isocoumarins

Sachin V Bhilare, *장민정, *윤소원

*LG Life Sciences *한양대 화학과*

N-Heterocyclic carbenes (NHCs) have attracted considerable attention from organic chemists. Their role as ancillary ligands for transition metals and their ability to efficiently catalyze a number of organic reactions, such as benzoin condensation, transesterification, aldol reaction, Stetter reaction, etc., have contributed significantly to the enormous interest in NHCs. There is also a growing awareness of their potential application as reagents in organic reactions.Recently, we have discovered an interesting NHC-catalyzed oxidative cyclization reactions which offer a simple and efficient route to the regioselective synthesis of phthalides and isocoumarins.

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Pd-Catalyzed Oxidative Coupling Reactions for the Synthesis of 5,6-Dihydrophenanthridines

김병석, 이동진, 윤소원

한양대 화학과

Recently, 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. C-H bond activation has been most efficiently achieved with the assistance of *N*-Ts amide as a directing group, and sequential C-C bond formation and intramolecular nucleophilic cyclization reaction occurred to provide a facile and efficient one-pot synthetic route to *N*-heterocyclic compounds.

한국화학회 THE KOREAN CHEMICAL SOCIETY

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Lewis Base-Catalyzed Acyl Cyanide Synthesis via Carbene Intermediate

최형호

경희대 화학과

The reactions of alkynyl aldehydes with trimethylsilyl cyanide in the presence of catalytic amount of a Lewis base such as TEA and DIPEA afforded the corresponding (E)-configurated, α,β-unsaturated acyl cyanides. TMSCN treated with TEA is effective reagent for generating allene species from alkynyl aldehydes, and this nucleophilic intermediate can be protonated by equimolar amount of ethanol, thereby promoting the efficient conversion into α,β-unsaturated acyl cyanides. Further investigations and applications of these acyl cyanide species are being actively pursued, such as 1,2- addition, 1,4-addition, or nucleophilic substitution reactions.

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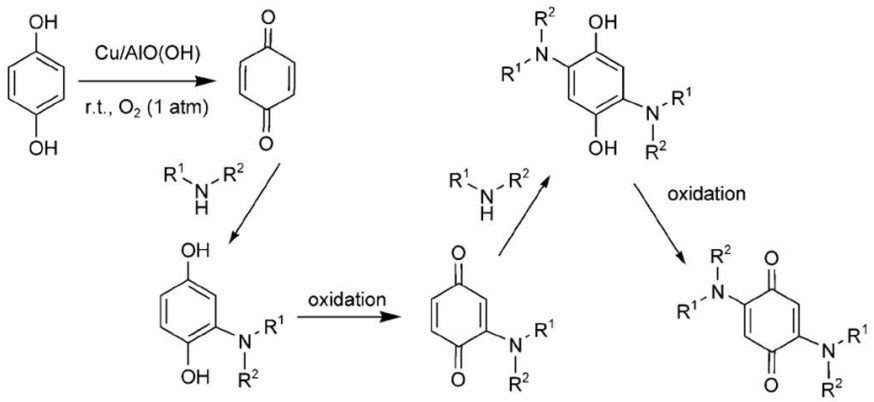
Synthesis of 2,5-diaminoquinones by one-pot copper catalyzed aerobic oxidation of hydroquinones and addition reaction of amines

김성진, 박재욱

포항공과대 화학과

Quinones are valuable compounds in nature and organic synthesis. In particular, aminoquinones have been studied for pigments and pharmaceuticals. The addition of amines to 1,4-benzoquinones is typical reaction for preparation of 2,5-diamino-1,4-benzoquinone. However, this method suffers from low reactivity of primary amines, and requires six equivalents of amines to complete the addition reactions. Herein, we report that the Cu/AlO(OH) is highly active and recyclable for the aerobic oxidation of a wide range of hydroquinones at room temperature. Furthermore, 2,5-diamino-1,4-benzoquinones were synthesized directly from hydroquinone and amines by a one-pot procedure consisting of the copper-catalyzed aerobic oxidation of hydroquinones and the double addition of amines to the resulting quinones (scheme 1).



Scheme 1. Direct synthesis of 2,5-diamino-1,4-benzoquinones using Cu/AlO(OH) under an oxygen atmosphere.

일시: 2010년 4월 29~30일(목~금) 2일간
장소: 송도컨벤시아
발표코드: **Ⅲ37P270포**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 금 10:30~12:30

Ru-catalyzed one-pot alcohol oxidation-Wittig reaction producing α,β-unsaturated esters

이은영, 박재욱

포항공과대 화학과

Ruthenium nanoparticles embedded in aluminum oxyhydroxide were applied to the one-pot oxidation-Wittig reaction. The Wittig reaction is an important reaction to provide α,β-unsaturated esters which are essential intermediates in natural product synthesis. By a one-pot process α,β-unsaturated esters were synthesized in high yields through the Ru-catalyzed oxidation of primary alcohols and the coupling of the resulting aldehydes and stabilized Wittig reagents. The method is applicable for aliphatic alcohols as well as benzylic ones, and does not require any additives such as base, co-catalyst, and ligand except oxygen.

Scheme 1. One-pot oxidation-Wittig reaction.

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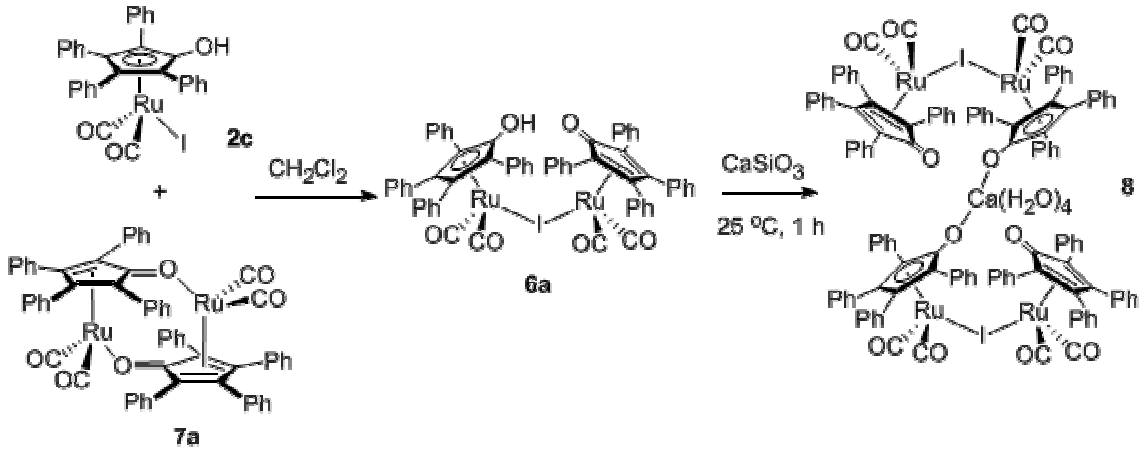
발표분야: 유기화학
발표종류: 포스터, 발표일시: 금 10:30~12:30

Formation of an Iodide-Bridged Diruthenium Complex from[(η^5-Ph_4C_4COH)$(CO)_2$RuI] and [(Ph_4C_4CO)$(CO)_2$Ru]$_2$: An Efficient Catalyst for Alcohol Oxidation with Ag_2O

도영실, 박재욱

포항공과대 화학과

Summary : Iodide-bridged diruthenium complexes, [(η^5-2,5-R_2-3,4-Ph_2C_4COH)$(CO)_2$Ru-(μ-I)-Ru$(CO)_2$(η^4-2,5-R_2-3,4-Ph_2C_4CO)] (6a,R=Ph; 6b,R=Me),were formed from the reaction of (η^5-2,5-R_2-3,4-Ph_2C_4COH)$(CO)_2$RuI (2c,R=Ph; 2d,R=Me) with [(2,5-R_2-3,4-Ph_2C_4CO)$(CO)_2$Ru]$_2$ (7a,R=Ph; 7b,R=Me). During the column purification of complex 6a, the complex [(η^4-Ph_4C_4CO)$(CO)_2$RuIRu(η^4-Ph_4C_4CO)$(CO)_2$]$_2$-Ca$(H_2O)_4$ 8 was obtained from the reaction of Ca originated from the silica gel. The structure of 8 was determined from the X-Ray analysis. The complexes 6a and 6b exhibited a high catalytic activity for the oxidation of alcohols with silver oxide (Ag_2O) at room temperature.(1) Do, Y.; Ko, S. B.; Hwang, I. C.; Lee, K. E.; Lee, S. W.; Park, J. Organometallics 2009, 28, 4624-4626.



Scheme 1. Reaction of (η^5-Ph_4C_4COH)Ru$(CO)_2$I with [(Ph_4C_4CO)Ru$(CO)_2$]$_2$

일시: 2010년 4월 29~30일(목~금) 2일간
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발표분야: 유기화학
발표종류: 포스터, 발표일시: 금 10:30~12:30

The efficient synthesis of perylenequinone core

김범태, *신영민, *송춘호, **한인철, **방성준, *조익수, *황기준

*전북대 생리활성물질연구소, 헬스케어기술개발사업 *전북대 화학과 **전북대 생리활성소재과학과*

Hypocrellin B is representative in a class of perylenequinones and has been utilized as an starting material for the further synthetic derivatization for novel lead compounds of photosensitizers in photodynamic therapy (PDT) against diverse cancers. This class of photosensitizers would be expected as an alternative for the Photofrin II which was only approved by FDA as the photosentitizer in PDT. However, hypocrellin B is natural product and supply-line is actually very limited in contrast of its urgent needs as a raw material. Therefore, as the first synthetic work, the efficient and economic synthetic methodology of perylenequinone core and ite derivatization were investigated by several approaches.

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발표분야: 유기화학
발표종류: 포스터, 발표일시: 금 10:30~12:30

Cyclo-Voltametric Study of of Novel Mono- and Dimeric LTAM Derivatives

노세정, 금삼록

고려대 소재화학과

Novel hetaryl leuco-TAM molecules, (2Z, 2E)-2,2-(2-phenyl- propane-1,3-diylidene)bis(1,3,3-trimethylindoline) derivatives, LT1-18 and 1-((1E,3Z)-1,3-bis(1,3,3-trimethylindolin-2-ylidene)propan-2-yl)-4-((1Z3E)-1,3-bis(1,3,3-trimethyl-indolin-2-ylidene)propan-2-yl)benzene derivatives, DLT1-3 were prepared from the reaction of excess Fischer base(FB) with correspondingly substituted benzaldehydes or terephthaldicarboxaldehydes. The electrochemical properties of heterocyclic leuco-TAM dyes, LT1-18 and DLT1-3, have been examined by CV. The CV of DLT 1-3 showed the doubly-oxidized peak in forming the TAM++ molecules.

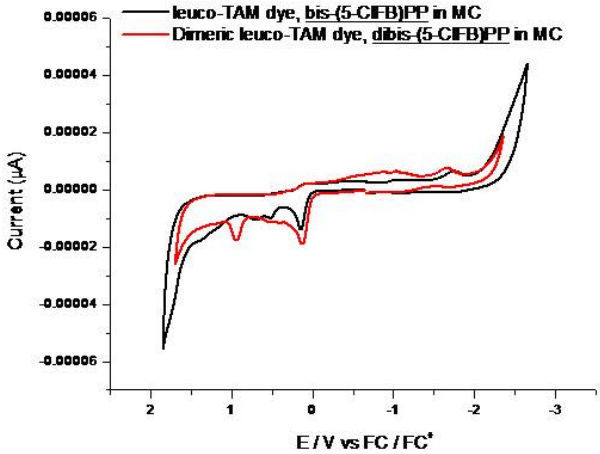

Figure 1. Cyclic voltammograms of Heterocyclic leuco-TAM, **LT2** (black line) and dimeric leuco-TAM **DLT2** (red line), at a platinum electrode (Φ) 1 mm in MC solution containing 0.1 M TBAP with v = 0.1 s1

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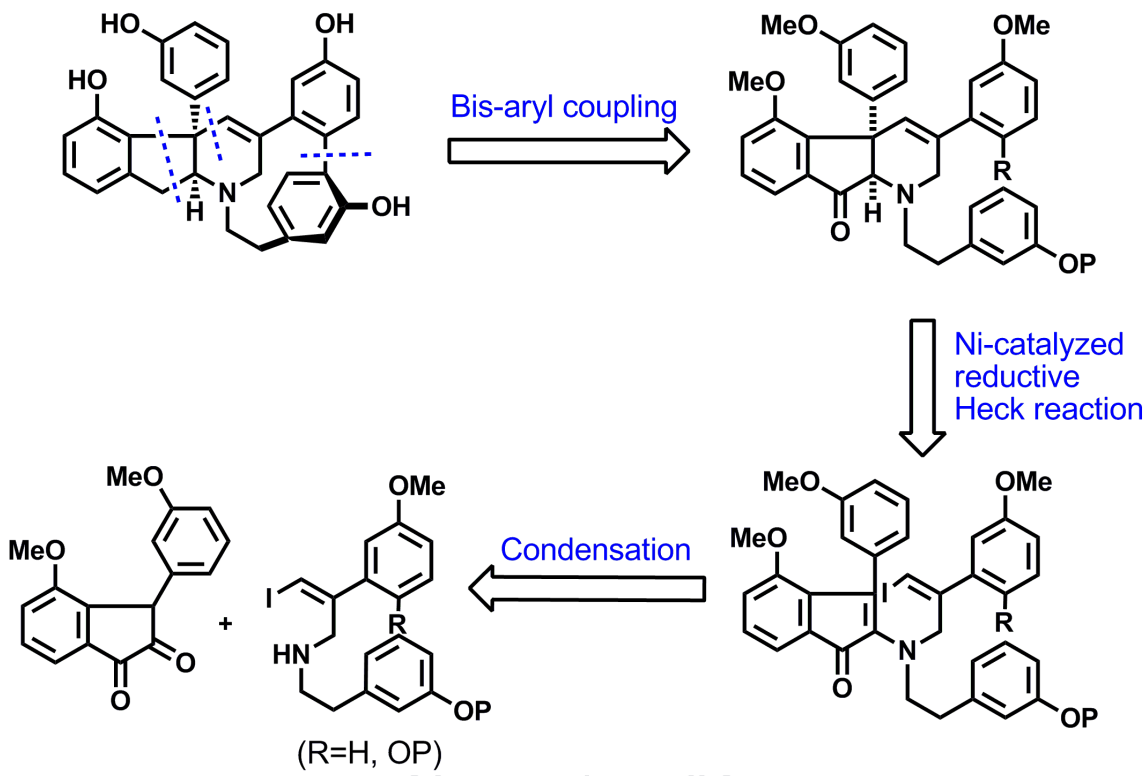
발표분야: 유기화학
발표종류: 포스터, 발표일시: 금 10:30~12:30

Studies Toward Total Synthesis of (-)-Haouamine A

안은혜, *이철범

*서울대 화학과 *서울대 화학부*

Haouamine A was isolated by Zubia and co-workers in 2003 from Aplidium haouarianum collected off in the southern coast of Spain. The molecule features an indeno tetrahydropyridine moiety that contains a diaryl quaternary center and an anti-bredt double bond. This tetrahydropyridine ring is further fused to a highly strained 11-membered paracyclophane that includes a bent aromatic ring. The marine alkaloid has an exquisitely selective anticancer activity against the human colon carcinoma cell line HT-29 with an IC50 of 0.1 μg/ml and against human prostate cancer cells with IC50 = 14.5 μg/ml. Presented here is our approach to haouamine A based on a concise and convergent synthetic plan. Highlights of our strategy are the use of a Ni-catalyzed asymmetric reductive Heck reaction and the formation of the paracyclophane moiety by conjoining two biaryl rings. So far, the formation of the indeno-tetrahydropyridine subunit has been achieved with high enantioselectivity by empoying chiral nitrogent ligands for the nickel catalyst. Currently, we are investigating the prospect of constructing the paracyclophane by connecting two aryl groups via a cross-coupling reaction or a benzyne intermediate. Details of the recent progress in our synthetic investigation will be described.



대한화학회 THE KOREAN CHEMICAL SOCIETY

일시: 2010년 4월 29~30일(목~금) 2일간
장소: 송도컨벤시아
발표코드: **Ⅳ38P112포**
발표분야: 의약화학
발표종류: 포스터, 발표일시: 금 15:00~17:00

A validation of solid phase extraction for purification of [C-11]6-OH-BTA-1 without HPLC

이상윤, 진혜영

가천의과학대 뇌과학연구소

Purpose[C-11]PIB has been a widely used PET agent for senile plaque quantification in patient with Alzheimer's disease and demented elderly, because of its excellent kinetic properties for brain imaging showing higher cortical [C-11]PIB binding than white matter and fast clearance in normal tissue. [C-11]PIB contains short lived radioisotope (half life = 20min) which can be major disadvantage for multiple injection daily basis. For other PET tracers (ex. Carfentanil, methionine, and so on) have been tried for rapid production without HPLC purification by using solid phase extraction cartridge, but all of them have significant physical properties between precursor and product (salt vs free base) so that we could separate precursor and byproducts from desired compound. In this report we tried to produce [C-11]PIB without HPLC by only using SPE cartridge for separation between free base species.ResultIn methylation step, we tried various amount and concentration of precursor and found that high concentration (1 mg precursor in 200 ul of solvent, 5000 ppm) can cause O-methylation (~10%) which can't be separated with SPE method, but lower concentration of precursor (500 ppm) was ideal only for N-methylation (confirmed with radio-TLC analysis) and showed similar yield comparing to high concentration. SPE separation also showed two advantages comparing to conventional method in total synthesis time (~20 min shorter) and yield (~ 20% better) with a very low chemical impurity (precursor) in our facility.ConclusionFirst trial for [C-11]PIB preparation with SPE purification method was performed. There are much improvement in synthesis time and radiochemical yield with any conflict in chemical impurities.

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발표분야: 의약화학
발표종류: 포스터, 발표일시: 금 15:00~17:00

Synthesis and SAR, and target protein identification of sulfonyl- and phosphoryl amidine compoundsas anti-resorptive agents

이명윤, *김진호, **김범태, ***정인화, *장석복, ****김성환, *****장성연

*연세대 화학과 *KAIST 화학과 **한국화학연구원 신약연구단 ***연세대 화학및의화학과 ****한국화학연구원 화학유전체 연구실 *****한국화학연구원 신물질 연구단*

A novel series of sulfonyl and phosphoryl amidines were synthesized efficiently via a Cu-catalyzed one pot reaction. Structure activity relationship studies led to the identification of potent anti-bone resorptive amidine derivatives with IC_{50} values less than 10 uM. Target protein identification of the amidine derivatives is under investigation with affinity chromatography and photoaffinity probes.

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장소: 송도컨벤시아
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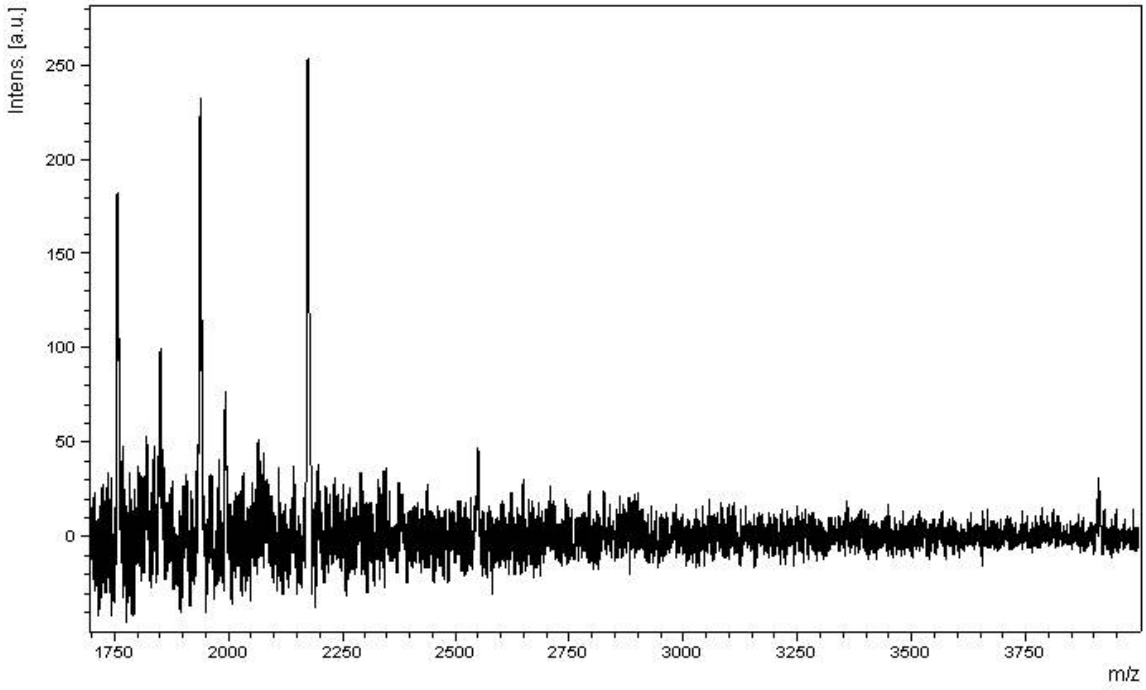
발표분야: 의약화학
발표종류: 포스터, 발표일시: 금 15:00~17:00

Hydrolysis by cleavage agent with Cu(II) cyclen against h-IAPP

정근홍, 정우영, 계영식, *박두한, *김한일

*육군사관학교학교 화학과 *삼육대 화학과*

Protein misfolding and aggregation have been linked with numerous fatal diseases including Type 2 diabetes mellitus(T2DM), which is manifested by reduction of β-cell mass. The amyloid is formed by the aggregation of the human islet amyloid polypeptide (h-IAPP) in the islet of Langerhans, resulting in cytotoxicity of β-cell. Co(III) complexes bearing macrocyclic structure have been proposed as therapeutic option. However, Cu(II) ion prevents h-IAPP from forming the β-sheet conformers. Therefore, we synthesized cleavage agent with Cu(II) cyclen to hydrolyze h-IAPP. The cleavage agent activity was judged by peptide fragments of h-IAPP. MALDI-TOF mass spectrum was obtained after incubation of h-IAPP with cleavage agent.



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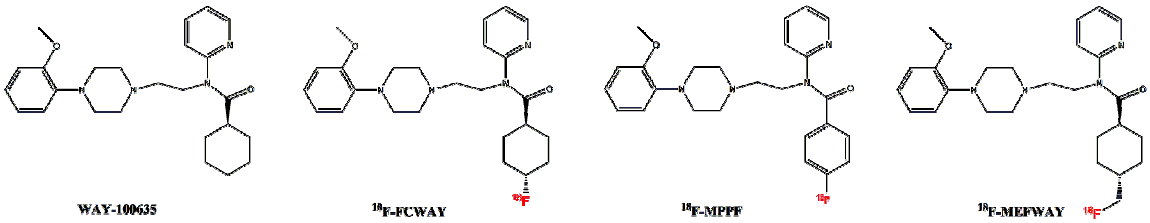
일시: 2010년 4월 29~30일(목~금) 2일간
장소: 송도컨벤시아
발표코드: **Ⅳ38P115포**
발표분야: 의약화학
발표종류: 포스터, 발표일시: 금 15:00~17:00

MicroPET study of WAY-100635 derivatives for PET imaging Brain 5-HT_{1A} receptors

최재용, *김철훈, **김병수, **김은정, **김정영, ***최태현, 유영훈

*연세대 핵의학과 *연세대 의과대학 약리학교실 **한국원자력의학원 방사성의약품연구팀 ***원자력의학원 국가방사선비상진료센터*

The serotonin (5-HT) system which is one of the most important neurotransmitter systems has been classified into seven subtypes. Among these subfamilies, disruption of 5-HT_{1A} receptors in the central nervous system is strongly associated in various neuropsychiatric disorders. 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. It is known that agonists bind to only the high affinity agonist state but antagonists bind to receptors in both their high and low-affinity state. Thereby a number of antagonist tracers have been developed as PET imaging agents on the basis of the WAY-100635. Here, we report that the comparative studies on WAY-100635 derivatives derivatives (i.e. ^{18}F-FCWAY, ^{18}F-MPPF, ^{18}F-MEFWAY) in a rat brain using microPET R4.



일시: 2010년 4월 29~30일(목~금) 2일간
장소: 송도컨벤시아
발표코드: **Ⅳ38P116포**
발표분야: 의약화학
발표종류: 포스터, 발표일시: 금 15:00~17:00

Arylpiperazine-containing pyrimidine 4-carboxamide derivatives as a potential antidepressant

김종엽, 강석연, *박우규, **배애님, ***김득준, 김정민, 이진화

*(주)녹십자 *한국화학연구원 약리활성연구센터 **KIST 생체과학연구본부 ***서울대 약학대*

Pyrimidine usually has good pharmacokinetic properties as a drug substance and considerable efforts have been devoted to develop pyrimidine derivatives into drug candidates. Arylpiperazine-containing pyrimidine 4-carboxamide derivatives were synthesized and evaluated for binding to serotonin receptors and transporter. Pyrimidine derivatives showed good antidepressant activity in FST (forced swimming test) animal model, and also displayed no appreciable inhibitory activity against CYP. Herein SAR studies of pyrimidine derivatives targeting serotonin receptors and transporter will be disclosed.

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발표종류: 포스터, 발표일시: 금 15:00~17:00

Synthesis and Biological Evaluation of New Arylpiperazine-Containing Pyrrole 3-Carboxamide Derivatives: Further Optimization for Targeting Serotonin 5-HT_{2A}, 5-HT_{2C}, and the Serotonin Transporter as a Potential Antidepressant

강석연, 박은정, 서희정, 김민주, *박우규, **배애님, ***김정민, 이진화

*(주)녹십자 *한국화학연구원 약리활성연구센터 **KIST 생체과학연구본부 ***(주) 녹십자*

In the continuing search as multiple target receptor for serotonin 5-HT_{2A}, 5-HT_{2C} and serotonin transporter, new arylpiperazine-containing pyrrole 3-carboxamide derivatives were synthesized and evaluated. Based on the previously reported lead, N-(3-(4-(2,3-dichlorophenyl)piperazin-1-yl)propyl)-1,2-dimethyl-5-phenyl-1*H*-pyrrole-3-carboxamide, structural modifications were accomplished for improvement of not only binding affinity against serotonin receptors and transporter, but also hERG channel inhibition. Along the line, the forced swimming tests as well as spontaneous locomotor activity tests were performed to distinguish between antidepressant activity and false-positive results using well-known animal model. As potential antidepressant agents, both 2,4-dimethyl-5-phenyl-1H-pyrrole-3-carboxamide and 5-tert-butyl-2-methyl-1H-pyrrole-3-carboxamide derivatives exhibited favorable *in vitro* and *in vivo* activities, warranting further investigation around these scaffolds.

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장소: 송도컨벤시아
발표코드: **Ⅳ38P118포**
발표분야: 의약화학
발표종류: 포스터, 발표일시: 금 15:00~17:00

Characterization and Cancer Cell Specific Binding Properties of Anti-EGFR Antibody Conjugated Quantum Dots

이정한, 송릿다

한국파스퇴르연구소 Nano/Bio Chemistry

Synthesis of biologically active antibody conjugated quantum dot (QD) has been of great importance in cellular imaging and diagnostics. Cetuximab (or Erbitux®) is the first monoclonal antibody drug which targets the epidermal growth factor receptor (EGFR) overexpressed in most cancer cells. In the present work, we investigated three different conjugation strategies to obtain the biologically functional QD-cetuximab conjugates for the tumor-specific imaging. Successful conjugation of cetuximab to QDs was achieved using PEG conjugated polymer-coated QDs and two long-chain heterobifunctional linkers, sulfo-LC-SPDP and sulfo-SMCC. The dissociation constant of the QD-cetuximab conjugates to EGFR was determined to be 0.61 ± 0.28 nM. The cancer cell-specific binding ability of the QD-cetuximab conjugates was evaluated in vitro, and the cellular internalization of the QD-cetuximab conjugates was clearly demonstrated in live cells by confocal microscopy. The cellular imaging experiments using the QD-cetuximab conjugates showed clear endocytosis pathway, which was evidenced by the co-localization of the QD-cetuximab conjugates with dye labeled transferrin. These results suggest that the QD-cetuximab conjugates as an imaging modality for tumor EGFR overexpression can be expected to provide important information on the expression levels of EGFR on the cancer cells.

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발표분야: 의약화학
발표종류: 포스터, 발표일시: 금 15:00~17:00

preparation of small molecule anticancer agents stabilizing G-quadruplex

한수진, 채정현, *김유리, **박현주

*성신여대 화학과 *성균관대 의약화학연구실/약학과 **성균관대 약학부*

Many Oncogenes have been shown to have G-quadruplex in their promoter regions and ligands which stabilize G-quadruplex could be developed as anticancer drugs. Based on the initial hit compounds discovered through virtual screening, we have designed the derivatives of two different types of heterocyclic compounds. Such compounds were synthesized either by simple substitution reaction of cyanuric chloride or by oxidative dimerization of substituted aminophenols. Some of the newly synthesized heterocyclic compounds showed increased activity in stabilizing G-quadruplex and improved cytotoxicity towards cancer cell lines.

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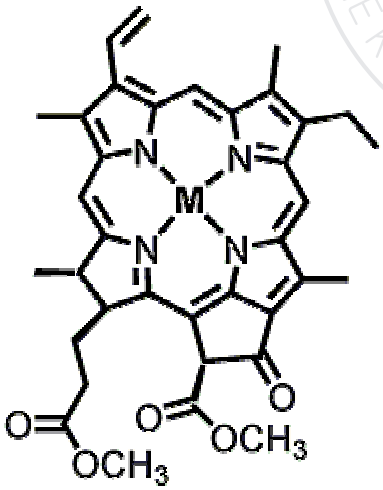
발표분야: 의약화학
발표종류: 포스터, 발표일시: 금 15:00~17:00

Synthesis and *in vitro* heavy-atom effect of transition metal complexes of methyl pheophorbide-a in photodynamic therapy

윤일, *박호성, **Cui Bing Cun, *심영기

*인제대 PDT 연구소 *인제대 나노공학부 **인제대 나노공학과*

Introduction of a heavy atom into photosensitizers improves the quantum yield of singlet oxygen in photodynamic therapy, which is called a heavy-atom effect. Transiton metal complexes of methyl pheophorbide-a were synthesized and their photodynamic therapy efficacy was confirmed by *in vitro* study.



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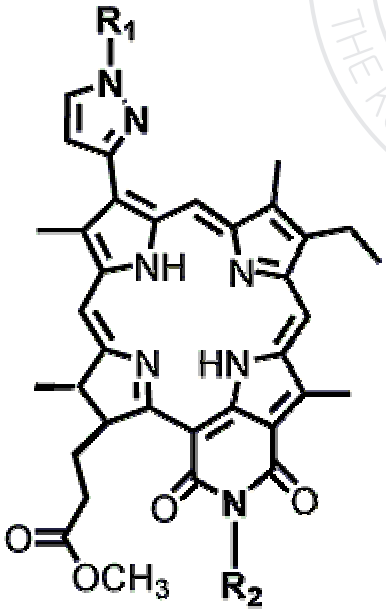
발표코드: **Ⅳ38P121포**
발표분야: 의약화학
발표종류: 포스터, 발표일시: 금 15:00~17:00

Synthesis and *in vitro* study of chlorin derivatives incorporating pyrazole unit in photodynamic therapy

윤일, *박호성, *심영기

*인제대 PDT 연구소 *인제대 나노공학부*

Pyrazoles have much attention as anticancer agents in biological system. Chlorin derivatives incorporating pyrazole unit were synthesized as new photosensitizers and their photodynamic therapy efficacy showed by *in vitro* study.



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발표종류: 포스터, 발표일시: 금 15:00~17:00

Synthesis and Biological Evaluation of Thiazolidinone Derivatives as Anti-inflammatory Agents

김희숙, *최경일, *신계정, 태진성, *남길수

*연세대 화학과 *KIST 생체과학연구본부*

In search of novel molecules for treating inflammatory disorders, we have found several hit compounds by *in silico* methods. Based on the hit compounds, we have designed new thiazolidinone derivatives, synthesized and evaluated their biological activities. The structure–activity relationships of the thiazolidinone derivatives have been elucidated.

THE KOREAN CHEMICAL SOCIETY

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Discovery of cyclicsulfonamide derivatives as 11 beta hydroxysteroid dehydrogenase 1 inhibitors

권성욱, 이재홍, *강승규, **김기영, ***이상달, *박지선, ****배명애, *****안진희

*고려대 화학과 *한국화학연구원 대사증후군치료제연구센터 **한국화학연구원 신약연구단 *** 한국화학연구원 분자약리연구팀 ****한국화학연구원 대사증후군치료제연구센타 *****한국화학연구원 대사성질환연구팀*

A new series of cyclic sulfonamide derivatives was synthesized and evaluated for their ability to inhibit 11 beta-HSD1. Cyclic sulfonamides with phenyl acetyl substituents at the 2-position showed nanomolar inhibitory activities. Among them, compound 4e exhibited a good in vitro inhibitory activity and selectivity toward human 11 beta-HSD2.

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Identification of cyclicsulfonamide derivatives with an acetamide group as 11 beta hydroxysteroid dehydrogenase 1 inhibitors

이재홍, *복주한, **강승규, ***김기영, ****이상달, *****강남숙, ******배명애, *******안진희

*고려대 화학과 *한국화학연구원 대사증후군센터 **한국화학연구원 대사증후군치료제연구센터 ***한국화학연구원 신약연구단 ****한국화학연구원 분자약리연구팀 *****한국화학연구원 신약플랫폼기술팀 분자설계 ******한국화학연구원 대사증후군치료제연구센타 *******한국화학연구원 대사성질환연구팀*

In the continuation of our 11 beta HSD1 inhibitor research, cyclic sulfonamide derivatives with an acetamide group at the 2-position was synthesized and evaluated for their abilities to inhibit 11 beta HSD1. Among this series, Compound 34 showed good in vitro activity toward human 11 beta HSD1, selectivity against 11 beta HSD2, metabolic stability, good PK and safety profiles (hERG and CYP). Also, a docking study explained the activity difference between human and mouse 11 beta HSD1.

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Solid-phase synthesis of 2-alkylamino substituted-1H-benzo[d]imidazole derivatives via thiol linker

김미선, 공영대

동국대 화학과

Solid-phase synthesis of combinatorial libraries has emerged as a powerful tool for efficient drug discovery process. Recently, we have been exploring the potential of resin-bound benzo[d]imidazole derivatives as a versatile intermediate for generation of drug-like heterocyclic compound libraries. Herein we would like to present a unique parallel synthetic method for combinatorial generation of 2-alkylamino substituted-1H-benzo[d]imidazole derivatives via thiol linker. The 2-alkylamino substituted-1H-benzo[d]imidazole derivatives have attracted much attention for their interesting various biological activity such as COX-2, 5-LO, and various receptors. 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-alkylamino substituted-1H-benzo[d]imidazole derivatives via BAL linker

장소영, 윤도경, 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]imidazole derivatives as a versatile intermediate for generation of drug-like heterocyclic compound libraries. Herein we would like to present novel solid-phase synthetic method for combinatorial generation of benzo[d]imidazole based library through resin-bound BAL linker. During about the past decade 2-amido/amine substituted benzo[d]imidazole derivatives have attracted much attention for their interesting biological activities such as COX-2, 5-LO, and various receptor antagonistics. The final compounds were obtained in good yields and high purities upon cleavage from the resins.

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발표종류: 포스터, 발표일시: 금 15:00~17:00

Solid-phase synthesis of 2-alkylamino substituted-1H-benzo[d]thiazole derivatives via BAL linker

심주용, 김미선, 공영대

동국대 화학과

Heterocyclic compounds are commonly used scaffolds on which pharmacophores are arranged to provide potent and selective drugs. As a part of our ongoing drug discovery program, we have been exploring the potential of resin-bound benzo[d]thiazole derivatives as a versatile intermediate for generation of drug-like heterocyclic compound libraries. Herein we would like to present a novel solid-phase synthetic method for combinatorial generation of benzo[d]thiazole based library through resin-bound BAL linker. The 2-alkylamino substituted-1H-benzo[d]thiazole derivatives have attracted much attention for their interesting biological activities such as COX-2, 5-LO, and various receptor antagonistics. The final compounds were obtained in good yields and high purities upon cleavage from the resins.

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Solid-phase parallel synthesis of 2-amido/amine substituted benzo[d]oxazole derivatives via BAL linker.

정세린, 양승주, 공영대

동국대 화학과

Solid-phase synthesis has become an extremely powerful technique for the generation of drug-like, small, organic molecule libraries in medicinal chemistry programs. Recently, we have been exploring the potential of resin-bound 2-amido/amine substituted 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. Herein we would like to present a novel solid-phase synthetic method for combinatorial generation of 2-amido/amine substituted benzo[d]oxazole library through resin-bound benzo[d]oxazole via BAL-linker.

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Sonic Hedgehog Homolog (SHH) Inhibitor Design by Pharmacophore Modeling and Virtual Screening

황성환, Sundarapandian, 이윤호, *이근우

*경상대 응용생명과학부 *경상대 생화학과*

Sonic hedgehog homolog (SHH) is involved in activation of the hedgehog pathway which has been implicated in the development of cancers in various organs. Cancer resulted from the transformation of adult stem cells into cancer stem cells would be occured by the abnormal activation of the pathway. Hence the inhibition of the hedgehog signaling by SHH inhibitor will provide an efficient therapy for a wide range of malignancies. In an aim to discover the new inhibitor candidates, we have accomplished a database of all the existing inhibitors and have generated a three dimensional chemical feature based pharmacophore model using Discovery Studio 2.5 software which would provide useful information for rational drug design.

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Isolation of Compounds from *Ficus erecta* var. sieboldii

박성환, 강혜정, 변상희, 이남호

제주대 화학과

Ficus erecta var. sieboldii KING (Moraceae) is a deciduous tree distributed in the southern region of Korea. This plant has been used as a folk medicine for the treatment of arthritis. In our continuing efforts to find biologically active compounds from plants in Jeju Island, we became interested in the extract of F. *erecta* stems. Repeated column chromatography of ethyl acetate soluble fractions in this extract led to the isolation six compounds such as β-sitosterol, *p*-hydroxybenzoic acid, stigmasterol, ethyl linoleate, *a*-amyrin acetate and vanillic acid. All of these compounds were isolated for the first time from F. *erecta*. These structures were elucidated on the basis spectroscopic data from 1D and/or 2D NMR studies as well as by comparison of the data with the literature values.

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Oxazole derivatives : SARIs (Serotonin Antagonist and Reuptake Inhibitors) as antidepressants

김나연, *이지은, 최기항, **박우규, ***추현아, ****배애님

*고려대 화학과 *인하대 화학과 **한국화학연구원 약리활성연구센터 ***KIST 생체과학연구부 ****KIST 생체과학연구본부*

Selective serotonin reuptake inhibitors (SSRIs) are the most widely used drugs. Recent studies suggest that SSRIs can be augmented by pre-treatment with 5-HT2A/2C antagonist. The human 5-HT2A/2C receptor has been implicated in several neurological conditions, and potent and selective 5-HT2A/2C ligands may have therapeutic potential for treatment of CNS diseases, such as depression. Therefore 5-HT2A and 5-HT2C receptors have been considered as reasonable targets for the improved treatment of depression. An oxazole derivative library, which consists of 62 compounds, was constructed. The library was biologically evaluated against serotonin receptors (5-HT2A/2C) and serotonin reuptake transporter. Some of the compounds show promising IC50 values and antidepressant-like effect in in vivo forced swimming test

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발표종류: 포스터, 발표일시: 금 15:00~17:00

Synthesis and anticancer activity of Deoxoartemisinin derivatives

김민규, *이용남, *임은영, *정만길

*연세대 화학과 *연세대 화학과*

Artemisinin 은 항말라리아 효과에 특별한 생물학적 활성을 지니고 있을 뿐 아니라 항암 효과가 있다고 보고된바 있다. Artemisinin 의 유도체인 artesunate, arteether, and artemeter 역시 melanoma, breast, ovarian, prostate, CNS, and renal cancer cell lines 에 대한 항암 효과를 갖는다. 또한 deoxoartemisinin 으로부터 합성된 monomer, dimer, and trimer 가운데 dimer 와 trimer 가 monomer 보다 더 좋은 항암효과를 갖는다. 본 연구실에서는 antitumor 에 대한 활성을 평가하기 위해 다양한 유도체를 합성하여 in Vitro 실험을 한 결과, deoxoartemisinin trimer 가 가장 좋은 항암효과를 갖는 것을 알아낼 수 있었다.

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Isoxazole Derivatives as Neuropathic Pain Therapy by T-type Calcium Channel Modulation

이지은, *이효선, **배애님, ***추현아

*인하대 화학과 *KIST 케모인포매틱스연구단 **KIST 생체과학연구본부 ***KIST 생체과학연구부*

T-type calcium channel is recently known as a good therapeutic target for the treatment of neuropathic pain. Since the withdrawal of mibefradil, a selective T-type calcium channel blocker, there have been a lot of efforts to develop T-type calcium channel blockers with new scaffolds and no side effect. We designed and synthesized novel isoxazole analogues as T-type calcium channel blockers. The synthesized isoxazoles were biologically evaluated against T-type calcium channel. Some of the compounds showed in vivo efficacy in neuropathic pain, which was compared with that of gabapentin, one of drugs on the market for the treatment of neuropathic pain. Selectivity, microsomal/plasma stability, and pharmacokinetic properties of the compounds with in vivo efficacy were further assessed.

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A Novel Inorganic Nanotube-Biopolymer Composite for Colon-Specific Anticancer Drug Delivery

Farrukh R. Ahmed, *K. E. Geckeler

*광주과학기술원 신소재공학과 *광주과학기술원 신소재공학과,나노바이오전자재료공학과, 의료시스템공학학제전공*

Inorganic nanotubes have found interest in several areas due to their specific application potential. Recently, halloysite nanotubes have received increased attention for their application in drug delivery and nanobiotechnology due to their low cytotoxicity and cost effectiveness. In the present study, halloysite nanotube-based composites have been prepared for simultaneous colon-specific delivery of 5-fluorouracil and folinic acid, the two most important drugs employed for the treatment of colorectal cancer. Three composites were prepared by coating the 5-fluorouracil-loaded nanotubes with folinic acid-conjugated chitosan. The different halloysite-nanotube composites were characterized by classical characterization techniques such as FT-IR spectroscopy, XRD, TEM, and TGA.

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Neolitsea aciculata Essential Oil Inhibits Drug-Resistant Skin Pathogen Growth and *Propionibacterium acnes*-Induced Inflammation in Murine Macrophage

김상숙, 강유미, 고하나, 이남호

제주대 화학과

This study was designed to analyze the chemical composition of *Neolitsea aciculata* essential oil (NAE) and to evaluate their biological activities. NAE were obtained by hydro-distillation of *N. aciculata* leaves collected in Jeju Island and were analyzed using gas chromatography equipped with Mass spectrometer detector. 1-Dodecen-3-yne (12.5%), calarene (11.5%) and elemol (9.5%) were identified as the major components in the NAE. Since acne vulgaris is the combined result of a bacterial infection and the inflammatory response to that infection, we examined whether NAE possessed antibacterial and anti-inflammatory activities against skin pathogens. As a result, NAE showed excellent antibacterial activities against drug-susceptible and -resistant *Propionibacterium acnes* and *Staphylococcus epidermidis*, which are acne-causing bacteria. In addition, NAE reduced the *Propionibacterium acnes*-induced secretion of tumor necrosis factor-α (TNF-α) and interleukin-8 (IL-8) in THP-1 cells, indicating its anti-inflammatory effects. In this study, NAE was also examined on DPPH radical scavenging activities, which showed moderate antioxidant activity (IC_{50}, 21.3 μL/mL). Taken together, we suggest that NAE may be an attractive candidate as an ingredient for skin care products.

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A novel synthesis and biological evaluation for Cardiovascular agent

임은영, 이용남, 정만길

연세대 화학과

Danshen is a representative oriental medicine used for the treatment of vascular disease. Magnesium lithospermate B (LAB) , an active component of Danshen, is a potent antioxidant. In structural aspects, it is tetramer of caffeic acid with seven phenolic hydroxyl groups. High molecular weight makes LAB unsuitable for further derivatization, so we sought a novel simplified lead compound with low molecular weight that retained high antioxidant effect. We describe the simple synthesis of novel stilbene derivatives based on LAB and determined the cardiovascular properties of each derivatives. The key synthetic strategies involved well-known Wadsworth-Horner-Emmons condensation and coupling reactions in high yields. All analogues were evaluated for DPPH radical scavenging effect, suppression of LPS-induced NO generation. Most of the trans-stilbene derivatives showed 2–3 times more radical-scavenging activity than resveratrol. They were also potent inhibitors of nitrite accumulation in LPS-stimulated microglia BV-2 cells. This result suggests that the prepared stilbene analogues exhibited a possibility for cardiovascular agent.

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synthesis of RGD-tagged Mesoporous silica nanoparticles and preliminary in vivo test

박주영, 김동욱

전북대 의과대학 핵의학과

Mesoporous silica nanoparticles (MSN) were synthesized by a self-assambly method. The MSN was conjugated with polyethylene glycol (Mw: 2000 or 3400) and then protected cRGDyk was attached to MSN-PEG. To radiolabel I-125, 4-aminophenol was conjugated to Cy5.5 and this was loaded in the pore of MSN-PEG-cRGDyk. X-ray diffraction (XRD) pattern of the crystal structure, nitrogen adsorption, TEM, and pore size distribution of MSN-PEG-cRGDyk were determined. In vitro cellular uptake was performed in human breast cancer (MDA-MB 231) cell line. For in vivo studies, 125I-Cy5.5 loaded MSN-PEG-cRGDyk was i.v. injected into the MDA-MB 231 xenografted mice.

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Synthesis and biological evaluation of phenylpyrazoles molecules as calcium channel blockers

노은선, *최경일, *남길수, 태진성

*연세대 화학과 *KIST 생체과학연구본부*

The T-type calcium channels are low voltage dependent calcium channels which have $Ca_{v3,1}(\alpha_{1G})$, $Ca_{v3,4}(\alpha_{1H})$ and $Ca_{3,3}(\alpha_{1I})$ subunits. Previously we have synthesized and evaluated α_{1G} channel inhibitory activities of pyrazole based molecules such as arylpiperazinylalkylaminomethylpyrazoles and arylpiperazinylethylcarbamoylmethylpyrazoles. To find more active compounds the structural optimization of previously found hit compounds was needed. In this study, a novel series of substituted phenylpyrazole scaffold was designed, synthesized and their α_{1G} and α_{1H} channel inhibitory activities were evaluated by FDSS system.

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Click Reaction of cMBP Peptide with Various [^{18}F]Fluoro-alkynes for Positron Emission Tomography

장승호, JADHAV VINOD HANMANT, 김동욱

전북대 핵의학과

Peptides make up a large part of the armamentarium available for the molecular imaging of cell-surface biomarkers. ^{18}F is particularly attractive for PET, as it has favorable decay characteristics ($t_{1/2}$ = 110 min). We report the use of the Cu(I)-catalyzed Huisgen cycloaddition, also known as a click reaction, to label cMBP peptide with [^{18}F]Fluoro-alkyne based aromatic, aliphatic and PEG by forming 1,2,3-triazole.

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발표코드: **Ⅳ38P140포**
발표분야: 의약화학
발표종류: 포스터, 발표일시: 금 15:00~17:00

Discovery of Selective and Potential T-type Calcium Channel Modulators: Synthesis and Biological Evaluation of Piperazine Analogues

신선미, *배애님, *이재균, **한소엽, *민선준, *조용서

*이화여대 화학 나노 과학과 *KIST 생명보건본부 뇌의약센터 **이화여대 화학과*

T-type calcium channels, also known as low-voltage-activated calcium channels play an important role in the regulation of neuronal excitability in the central and peripheral nervous system. Recent studies showed that modulation of T-type calcium channels involves several pathophysiological diseases such as epilepsy, pain, hypertension, congestive heart failure and cancer. Therefore, potent and selective inhibitors are requested to explore the fundamental function of T-type calcium channels in such disease states.Based on three dimensional ligand-based pharmacophore model, we have designed and synthesized a series of new piperazine derivatives. Their inhibitory activities on T-type calcium channels have been evaluated using in-vitro assay against α1G and α1H subtypes by FDSS screening system. Furthermore, we have selected the compounds with high potencies and then analyzed their selectivities over hERG and N-type calcium channels as well as their stabilities in both rat plasma and human hepatic microsomes.

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Compounds with elastase inhibition and free radical scavenging acivities from *Callistemon lanceolatus*

김주희, 김정은, 이남호

제주대 화학과

Bioassay-guided investigation of the stems of *Callistemon Iannceolatus* led to the isolation of five compounds such as betulinic acid, pyracrenic acid, arjunolic acid, catechin, and piceatannol. Their structures were elucidated on the basis of spectral studies as well as by comparison with literature data. Elastase inhibition and DPPH radical scavenging activities were investigated for the isolated compounds. Among these, pyracrenic acid was identified as a potent elastase inhibitor with an IC_{50} value of 1.5 ug/mL, more active than the control compound, oleanolic acid (IC_{50} = 3.0 ug/mL). With regard to antioxidative studies, strong to moderate DPPH radical scavenging activities were observed with pyracrenic acid, catechin and piceatanol.

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Novel Indolyl Acrylic Acid Derivatives as Potent Inhibitors of Diacylglycerol Acyltransferse

이보아, 정화영, *김일순, **권정진, **이경, ***이현선, 최용석

*고려대 생명과학대학 *배재대 생화학과 **동국대 바이오시스템대학 ***한국생명공학연구원 분자암연구센터*

Triglyceride (TG) is a major form of stored energy in eukaryotes, and it is synthesized primarily through acyl CoA : diacylglycerol acyltransferase (DGAT) reaction that catalyzes the final and the only committed step in the glycerol phosphate pathway involving in the biosynthesis pathways of TG within the insulin-sensitive tissues including the adipose tissue, skeletal muscles, liver, and the β-cells of the pancreas. TG synthesis is important in mammals for energy storage in the adipose tissue and muscle, fat absorption in the intestine, and the assembly of lipoprotein in the liver and in the small intestine as well. As TG is also essential for the accumulation of adipose tissue in the body, inhibition of TG synthesis may reduce the incidence of obesity and its related diseases. Recently, it has been reported that diet-induced obesity caused by high fat diet could be effectively inhibited in DGAT-1 knock-down mice, and abnormal glucose metabolism was improved by increase of the susceptibility of insulin and leptin, the dietary hormones. As inhibition of DAGT has emerged as a therapeutic target for inhibiting TG synthesis, a potent DGAT inhibitors would be useful for the treatment of metabolic diseases. In the search of novel DGAT inhibitors, it was found that novel indolyl acrylic acid derivatives showed potent DGAT inhibitory effect. Herein, the structure-activity relationships of the indolyl acrylic acid derivatives will be presented.

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발표종류: 포스터, 발표일시: 금 15:00~17:00

Synthesis and evaluation of 5,6-Dihydro-pyrrolo[3,4-b]pyridin-7-one derivatives as MCH receptor 1 antagonist

임채조, 왕수미, 김지영, 서무영, 김낙정, 이규양, *송석진

*한국화학연구원 대사증후군치료제연구센터 *유유제약 중앙연구소*

The melanin-concentrating hormone receptor (MCH-R1) as a cyclic 19-amino acid neuropeptide is one of the most promising targets in 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 investigated the influence of various aryl substituents at 2-position. As a result, we have found that several compounds exhibited high MCH-R1 binding affinity in vitro assay. The details of synthesis and binding affinity will be discussed.

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Synthesis and evaluation of benzofuran derivatives as MCH receptor 1 antagonist

임채조, *이은경, 김지영, 김낙정, 이규양, **송석진

*한국화학연구원 대사증후군치료제연구센터 *과학기술연합대학원대 의약및 약품화학 **유유제약 중앙연구소*

Antagonists of the melanin-concentrating hormone receptor (MCH-R1) have great potential utility for the treatment of obesity. As part of our ongoing project in the development of MCH-R1 antagonists, a series of benzofuran carboxylic amide derivatives were designed, synthesized and evaluated. The benzofuran derivatives were easily prepared from the coupling of benzofuran carboxylic acid with arylpiperidine alkyl amine. Among them, several compounds showed excellent MCH-R1 binding affinity in vitro assay. The detailed results of structure-activity relationships (SAR) will be presented.

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발표종류: 포스터, 발표일시: 금 15:00~17:00

Synthesis and Biological Evaluation of N-Hetroaryl-3-Phenylsulfonyl-2-hydroxy-2-methyl propionamide derivatives As Androgen receptor Antagonists.

김준영, 김낙정, 이규양, 서지희, 임채조, *강남숙, **김성환

*한국화학연구원 대사증후군치료제연구센터 *한국화학연구원 신약플랫폼기술팀 분자설계 **한국화학연구원 화학유전체 연구실*

Carcinoma of the prostate(Cap) is the second leading cause of cancer related death in men. The androgen receptor(AR) is a ligand binding transcription factor in the nuclear hormone receptor super family. The AR antagonists are useful in treatment of prostate cancer, benign prostate hyperplasia, alopecia, and acne.A series of N-Heteroaryl-3-phenylsulfonyl propionamide derivatives has been synthesized and biological evaluatied using cell based assay(LNCap/PC-3 cells). The synthetic method and structure-activity realationships results will be discussed in detail.

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A Novel Class of DAXX nuclear export inhibitors;Synthesis and biological evaluations of naphtho[1,2-b]thiophene derivatives

이서현, 서지희, 이규양

한국화학연구원 대사증후군치료제연구센터

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 our efforts to find new scaffolds of DAXX nuclear export inhibitors as effective anti-ischemic agents, we have designed and synthesized a series of naphtho[1,2-b]thiophene derivatives.Synthesized compounds were biologically evaluated using in vitro H9c2 cell.Pharmacological activities correlated with their structures will be presented.

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Synthesis & Evaluation of 4-Aryl-2-anilino-thiazole derivatives as Androgen Receptor Antagonists.

김수희, *김낙정, **김성환, *이규양, *서지희, *임채조

*창원대 화학과 *한국화학연구원 대사증후군치료제연구센터 **한국화학연구원 화학유전체 연구실*

Androgen receptor(AR) is an important member of the superfamily of nuclear hormone receptors that functions as ligand-dependent regulators of transcription.The AR antagonist 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 4-Aryl-2-anilinothiazole derivatives.Among them, some of these compounds exhibited a potent activity in cell based assay. The details of synthesis and biological efficacy will be presented.

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Discovery of N-hydroxyl urea derivatives as b-raf kinase inhibitors

이강진, *정희정, *이종국, **한선영, *하재두, ***류재욱, *김형래, *조성윤, ****심태보

*충남대 화학과 *한국화학연구원 난치성질환치료제연구센터 **한국화학연구원 약리활성연구센터 ***한국화학연구원 바이오소재연구센터 ****KIST 생체과학연구본부*

Map kinases consist of Ras/Raf/MEK/ERK signal transduction pathway functioning in cell proliferation, differentiation, and survival, and play a critical role in many aspects of tumorigenesis. B-raf, a member of serine/threonine protein kinases that involved in Ras-mitogen activated protein kinase (MAPK) signal transduction pathway has been shown to be mutated in 66% of malignant melanoma, 40-70% of papillary thyroid carcinoma and 12 % of colon carcinoma.In an effort to search of b-raf inhibitors, N-hydroxyl urea derivatives as a novel series of compounds were synthesized and evaluated toward the b-raf kinase inhibitory activity. Some of compounds showed moderate activity as b-raf inhibitor in cell-based assay.

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Development of Classification Model for hERG Ion-channel Inhibitors using SVM Method

강신문, *남기엽, **노경태

*(사)분자설계연구소 신약개발 *(사)분자설계연구소 신약개발실 **연세대 생명공학과*

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. As one of these attempts, 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 setting, are still far from solved. The two problems have been shown to be crucial to the efficiency and accuracy of SVM classification. In particular, the feature selection and optimal SVM parameters setting influence each other, which indicates that they should be dealt with simultaneously. In this account, we present an integrated practical solution, in which genetic-based algorithm (GA) is used for feature selection and grid search (GS) method for parameters optimization. hERG ion-channel inhibitor classification models of ADME/T related properties has been built for assessing and testing the proposed GA-GS-SVM. We generated 6 different models that are 3 different single models and 3 different ensemble models using training set - 1891 compounds and validated with external test set – 174 compounds. We compared single model with ensemble model to solve data imbalance problems. It was able to improve accuracy of prediction to use ensemble model.

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Synthesis and Biological Evaluation of 2-Aryl-5-substituted phenyl-2H-pyridazinone Derivatives as Androgen Receptor Antagonists

윤부순, *김낙정, **강남숙, ***김성환, *이규양, *서지희, *임채조

*한국화학연구원 화학과 *한국화학연구원 대사증후군치료제연구센터 **한국화학연구원 분자설계실 ***한국화학연구원 화학유전체 연구실*

Androgen Receptor (AR) is a important member of the superfamily of nuclear hormone receptor that functions as ligand dependent regulators of transcription. The AR antagonists are useful in treatment of prostate cancer.A series of 2-Aryl-5-substituted phenyl-2H-pyridazinone derivatives were synthesized and biological evaluated using cell based assay (LNCaP/PC-3 cell) for androgen antagonist activities. Among these compounds, several was found to have potent activity.

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Development of Prediction Method for CYP3A4 inhibitions by Quantum-Mechanical Calculations

이주연, *강남숙, **강영기

*한국화학연구원 신약플랫폼기술팀 *한국화학연구원 분자설계실 **충북대 화학과*

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The active site of the cytochrome P450 (CYP450) is composed of an iron(III)-porphyrin moiety.

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Discovery of Cannabinoid-1 Receptor Antagonists by Virtual Screening

이길남, 강남숙

한국화학연구원 신약플랫폼기술팀 분자설계

CB1 is one of cannabinoid receptor subtypes, can be detected mainly brain but also in the lungs, liver and kidney recently potential target for obesity and drug addiction. we tried to find new scaffold for CB1 antagonist using virtual screening. We first analyzed structural features for the known Cannabinoid1 receptor antagonists and then, we built the pharmacophore models using HipHop concept and carried out the docking study based on our homology CB1 3D structure.

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Synthesis of triclosan derivatives as antibacterial agents

inna slynko, *Deepak Bhattarai, **배애님, ***금교창

*KIST 뇌의약센터 *과학기술연합대학원대 organic chemistry **KIST 생체과학연구본부 ***KIST 케모인포메틱스연구센터*

The biphenyl ether antibacterial agent, triclosan, shows broad- spectrum antibacterial activity by targeting the fatty acid biosynthetic pathway through inhibition of enoyl-acyl carrier protein reductase (ENR) and provides a potential scaffold for the development of new broad spectrum antibiotics. The methods of rational drug design for the development of inhibitors were applied by using of crystal structures for FabI and we synthesize the promising derivatives, tested them for their inhibitory activity against various bacteria and Mycobacterium tuberculosis. Some of these compounds showed good activity of low MIC values against Staphylococcus aureu, Enterobacter cloacae, Mycobacterium tuberculosis, in in-vitro assay.

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Novel benzenesulfonamide derivatives; their synthesis and biological activities as T-type calcium channel blocker.

이주현, *강순방, 정낙철, *김유승, *금교창

*고려대 화학과 *KIST 생명보건본부 뇌의약센터*

T-type calcium channels are important regulators of neuronal excitation, and are essential mediators of hormone secretion. However, T-type calcium channel hyperactivity has been linked to neurological disorders such as epilepsy and neuropathic pain. Mibefradil is the first marketed selective T-type calcium channel blocker. So, We have particullary studied the structure of Mibefradil for the development of novel T-type calcium channel blockers. A series of novel benzenesulfonamide derivatives were designed and synthesized based on the 3D pharmacophore model constructed with known T-type Ca2+ channel blockers. The compounds were studied for the evaluation of in-vitro inhibitory activities with a1G and a1H channel in FDSS assay system, and the selectivity against hERG channel. Some selected compounds were further studies PK and in-vivo activity using animal model. So, we'll discuss the structure-activity relationship.

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Synthesis of Water soluble polymer coated Gadolinium Oxide Nanoparticles for Magnetic Resonance Image

양은지, *Patel Mehulkumar, **김희경, *김태정

*경북대 나노과학기술학과 *경북대 응용화학과 **경북대 의용생체공학과*

Magnetic resonance imaging (MRI) is a very important noninvasive technique that is used to diagnose diseases. The diagnosis of diseases through MRI is further improved by using the MRI contrast agent. Two types of MRI contrast agents have been developed so far. One is the dextran coated superparamagnetic iron oxide nanoparticle, which possesses a very large transverse relaxivity (r2) of water proton of 100−200 s−1 mM−1 (T2 MRI contrast agent). The other is the paramagnetic Gd(III)−chelate that possesses a longitudinal relaxivity (r1) of water proton of 3−5 s−1 mM−1 (T1 MRI contrast agent). Gadolinium oxide nanoparticles could be one of such candidates because they can have larger r1 values than Gd(III)−chelates, depending on their particle diameter. In this work, we present synthesis of water soluble polymer coated gadolinium oxide nanoparticles with average particle diameters that range from 2 – 5 nm.

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DOTA Conjugated Tranexamic acid(ester) Gd-complexes: For Fine Tuning the Magnetic Resonance Imaging Properties

구성욱, *APURI SATYENDER, **김희경, *김태정

*경북대 응용화학과 *경북대 응용화학과 **경북대 의용생체공학과*

A series of DOTA conjugated of tranexamic acid, its esters, and their Gd(III) complexes of type[Gd(L)(H2O)]·nH_2O were synthesized and characterized. All Gd complexes exhibit enhanced R_1 relaxivity compared with Gd-DOTA(DOTAREM®). Highest R_1 was observed for [Gd(L3)(H_2O)](6.75 $mM^{-1}s^{-1}$). Potentiality of Gd(III) complexes(1-3) as contrast agent for magnetic resonance imaging (MRI CA) was investigated by measuring some relevant physicochemical properties such as (i) the protonation constants (ii) thermodynamic and conditional stability constants (iii) the selectivity(pGd) of 1-3 for the Gd(III) ion over the endogenous metal ions such as Zn(II), Ca(II), and Cu(III).

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Design and synthesis of a new Series of Iodo-phosphorylated scaffolds as potential x-ray contrast agents

APURI SATYENDER, *구성욱, 김태정

*경북대 응용화학과 *경북대 응용화학과*

X-ray imaging is a well known and extremely valuable tool for the early detection and diagnosis of various disease states in the human body and the use of contrast agents for image enhancement in medical x-ray imaging procedures are wide spread. Of the known radiographic agents, iodinated compounds have become standard contrast agents in the best sense because millions of patients suffering from conceivable diseases have received these contrast agents. Despite of numerous advantages associated with iodine based compounds; they have certain limitations like high viscosity, osmolity and low hydrophilicity. In order to overcome these drawbacks we intended to synthesize new scaffolds of iodinated compounds by introducing phosphate functionality. Based upon our ideology, herein we report the synthesis of a new series of iodo-phosphorylated compounds as potential radiographic agents.

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Development of Novel Fluorescent Xanthines as Kinase Inhibitors

김동희

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Kinase 를 목표물로 하는 암치료에 있어 변이된 암세포를 진단하는 것과 Kinase 를 저해하는 것은 중요하다. 특히 암세포를 진단하는 데 있어 형광을 이용하면 동위원소 등 방사능을 이용하는 방법보다 인체에 해가 없이 안전하게 진단할 수 있는 장점이 있다. 암세포를 진단하고 저해하는데 있어 기존에는 형광물질과 저해제를 따로 합성하여 연결하였는데 기존에 시도된 방법대로 각각 만든 두 가지 물질을 붙이면 분자량과 그 크기가 상당히 크기 때문에 세포 투과성 등에 문제가 발생하였다. 그러나 한 물질에 두 기능이 모두 존재한다면 이러한 단점을 극복할 수 있다. 또, 저해제는 암질병과 관련된 특정 Kinase 에만 선택적으로 붙기 때문에 그 물질 자체가 형광을 낸다면 변이된 암세포만 선택적으로 진단할 수 있는 장점이 있다. 우리 연구에서는 Kinase 의 3 차원 구조를 바탕으로 xanthine 을 출발물질로 하여 효과적인 합성방법으로 다양하고 우수한 형광 Kinase 저해제의 유도체를 합성하고 측정 등 일련의 과정을 수행하여 그 결과에 대해 발표하려 한다.

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Gd-complexes DTPA-bis(amide) conjugates of phosphorylated cyclohexane derivatives for magnetic resonance imaging

Patel Mehulkumar, *양은지, **김희경, 김태정

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Magnetic resonance imaging (MRI) possesses an unsurpassed potential for the exploitation of intrinsic tissue and structural differences visualized as image contrast by using a wide variety of pulse sequences. Typically, MRI contrast depends on endogenous differences in water content and relaxation time in the tissue of interest. The specificity and sensitivity of MR imaging can be further enhanced by the utilization of contrast agents based on paramagnetic metals such as gadolinium. We have recently reported Gd-complexes of DTPA-bis(amide) conjugates of tranexamic esters exhibit much higher r1 relaxivity than Omniscan®. In this regard, we anticipated that further modification of cyclohexane moiety in these ligands. Herein, we report the synthesis of Gd-complexes DTPA-bis(amide) conjugates of phosphorylated cyclohexane derivatives and their evaluation as potential MRI contrast agents.

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Characteristics of Tyrosinase Inhibitory Extract from *Pterocladia tenuis*

한충훈, 이선주, 이은숙, *오한솔, *정덕상

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Tyrosinase inhibitory activities of 4 kinds of seaweed, *Pterocladia tenuis, Lomentaria catenata, Gymnogongrus flabelliformis* and *Hypnea japonica* were determined using commercially available mushroom tyrosinase in an in vitro assay system. Ethanolic extracts(IC_{50}=111.66 μg/mL) of *Hypnea japonica* was more effective in the tyrosinase activity then other seaweed. Tyrosinase inhibitory activity of EtOAc extract from *Pterocladia tenuis* was 69.87% at a concentration of 1000 μg/mL.

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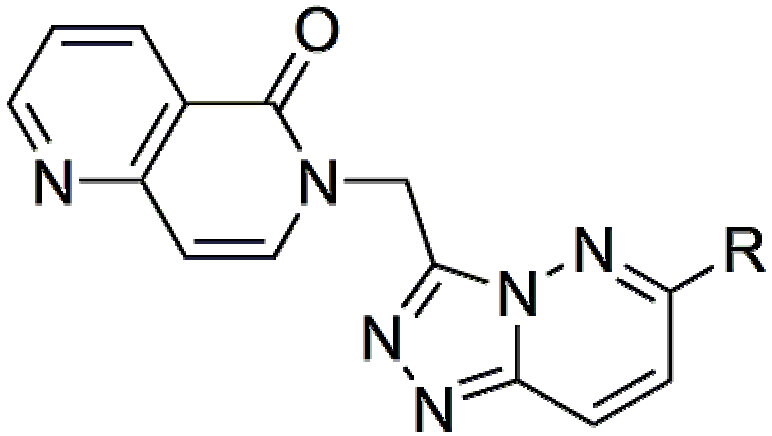
Discovery of 1,6-naphthyridin-5(6H)-one derivatives with [1,2,4]triazolo[4,3-b] pyridazine as inhibitors of c-Met receptor tyrosine kinase

양은혜, *김정근, **윤우섭, 이종국, ***한선영, 조성윤, ****이정옥, 김형래, 하재두

*한국화학연구원 난치성질환치료제연구센터 *고려대 화학과 **레고캠바이오 화학과 ***한국화학연구원 약리활성연구센터 ****한국화학연구원 항암제연구센터*

c-Met is a glycosylated, heterodimeric receptor tyrosine kinase, which is primarily expressed on epithelial and endothelial cells. The activation of c-Met is ligand dependent with the natural ligand being hepatocyte growth factor (HGF) also known as scatter factor (SF). The binding of HGF to c-Met receptor results in receptor autophosphorylation and upregulation of Met kinase activity, activating a complex downstream signaling pathway. Because deregulation of c-Met signaling contributes to oncogenesis and tumor progression in several human cancers and promotes aggressive cellular invasiveness that is strongly linked to tumor metastasis, c-Met is an attractive target for small molecule drug discovery. Herein, we report the discovery of a related series of 6-([1,2,4]triazolo[4,3-b]pyridazin-3-ylmethyl)-1,6-naphthyridin-5(6H)-one which demonstrate nanomolar inhibition of c-Met kinase activity.



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Synthesis and Activity of Tryptanthrin Analogs as Anti-Tuberculosis Agents

황재민, *조상래, *오태권, **Anna Upton, **Takushi Kaneko, **Christopher Cooper, **Zhenkun Ma, ***이상호, ****윤창수, *****김필호

*한국화학연구원 난치성치료제연구센터 *연세대 의과대학 **The Global Alliance for TB Drug Development ***한국화학연구원 신약연구단 ****한국화학연구원 신물질연구단 난치성질환치료제연구센터 *****한국화학연구원 난치성질환치료제연구센터*

Tuberculosis (TB) kills more than two million people per year worldwide. For the last four decades, there have been no novel TB drugs developed. Although the main burden of TB still remains on developing countries, developed countries are not immune to the possible outbreak of TB pandemic. The emergence of multi-drug resistant (MDR) and extensively-drug resistant (XDR)-TB makes it more challenging to cure TB. Thus, we need to develop novel TB drugs to overcome the current TB burden. The Global Alliance for TB Drug Development (GATB) has been one of the leading institutes to manage TB drug development programs worldwide. Recently KRICT and GATB undertook a new program centered around a natural product, tryptanthrin. Tryptanthrin has been known to be active against *Mycobacterium tuberculosis* (Mtb), which causes TB. We will present our strategies to undertake TB drug discovery program with tryptanthrin and its derivatives as well as our synthetic efforts and biological data.

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Discovery of Natural Products Active Against *Mycobacterium tuberculosis*

김수현, *이용섭, **조상래, ***이종석, **오태권, ****김필호

*경희대 기초약학과 *경희대 약학과 **연세대 의과대학 ***국제결핵연구소 기초연구부 ****한국화학연구원 난치성질환치료제연구센터*

Tuberculosis (TB) still remains one of the most deadly infectious diseases to human beings. Current TB regimen includes cornerstone drugs derived from natural products such as rifampicin and isoniazid. In our program aiming at the discovery of anti-tubercular natural products from soil bacteria, we have used assay-guided fractionations. Extract Collection of Useful Microorganism (ECUM) has been instrumental to provide us with second metabolite samples from *Streptomyces*. We will present the strategies used and update on the structure elucidation of anti-tubercular natural products.

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Bromomyrothenone B from a Marine Isolate of the Fungus Trichoderma viride

fengzhile, nenkep viviane nadeg, yangguohua, siwe noundou xavier, Leutou Alain Simplic, 윤금자, 손병화, *최홍대

*부경대 화학과 *동의대 화학과*

As part of an effort to discover biologically active natural products from marine sources, we investigated the bioactive secondary metabolites of a marine isolate of the fungus Trichoderma viride. The fungal strain, T. viride, was isolated from the surface of the edible marine red alga Gracilaria verrucosa, collected at Yokji Island of Gyeongnam, Korea in 2008, and identified as T. viride based on 18S rRNA analyses (SolGent Co., Ltd., Daejeon, Korea), identities of 100%. The cultured medium of T. viride was filtered through cheesecloth to give mycelium and broth. The filtered broth was extracted with EtOAc to afford broth extract (1.2 g), which was subjected to silica gel flash chromatography and purified by repeated silica gel flash chromatography (n-hexane in ethyl acetate) and HPLC (ODS-A, MeOH-H2O = 5:1) to yield bromomyrothenone B (9.3mg). The stereostructure of bromomyrothenone B was elucidated by combined physicochemical data analyses including circular dichroism (CD).

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Botrytinone from the Marine-Derived Fungus Rhizopus stolonifer

nenkep viviane nadeg, yangguohua, siwe noundou xavier, Leutou Alain Simplic, fengzhile, 윤금자, 손병화, *최홍대

*부경대 화학과 *동의대 화학과*

As part of an effort to discover biologically active natural products from marine sources, we investigated the bioactive secondary metabolites of a marine isolate of the fungus Rhizopus stolonifer, isolated from the surface of the edible marine brown alga Sargassum horneri, collected at Yokji Island of Gyeongnam, Korea in 2008, and identified as R. stolonifer based on 18S rRNA analyses (SolGent Co., Ltd., Daejeon, Korea), identities of 100%. The cultured medium of R. stolonifer was filtered through cheesecloth to give mycelium and broth. The filtered broth was extracted with EtOAc to afford broth extract (1.0 g). The broth extract of R. stolonifer was subjected to silica gel flash chromatography. Elution was performed with n-hexane - EtOAc (stepwise, 0 - 100 % EtOAc) to yield four fractions. Fraction 3 on medium pressure liquid chromatography (MPLC) (ODS) by elution with H2O-MeOH (from 1:1 to 1:5) afforded crude botrytinone, which was further purified by HPLC (YMC, ODS-A) utilizing a 30 min gradient program of 50% to 100% MeOH in H2O to furnish botrytinone (6.6 mg). The molecular structures and absolute stereochemistry of botrytinone was determined from chemical and physicochemical evidence, including quantum chemistry calculations, X-ray analysis, and the circular dichroism (CD) exciton chirality method.

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Clavatol from the Marine-Derived Fungus Cladosporium sp.

yangguohua, siwe noundou xavier, Leutou Alain Simplic, fengzhile, nenkep viviane nadeg,
윤금자, 손병화, *최홍대

*부경대 화학과 *동의대 화학과*

Our screening assays were designed to identify antimicrobial compounds that are active against Staphylococcus aureus, methicillin-resistant S. aureus (MRSA), and multidrug-resistant S. aureus (MDRSA). We investigated antimicrobial activity from the fungal extracts, and a crude mycelium extract of Cladosporium sp. was found to be active in the S. aureus, MRSA, and MDRSA screen. Assay-guided isolation of antimicrobial compounds from the mycelium extract to yield clavatol. The structure of clavatol was determined on the basis of the physicochemical data. Clavatol showed moderate antibacterial activity against S. aureus, MRSA, and MDRSA with minimum inhibitory concentration (MIC) values of 62.5, 62.5, 31.0 μg/mL, respectively. Calvatol also exhibited a UV-A protection activity with ED50 values of 227.0 μM, indicating that clavatol was more potent than the positive control, oxybenzone (ED50 values of 350 μM), a common sunscreen agent.

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QSAR predictive models for hERG inhibition

김준형, 강신명, 채종학, 강남숙

한국화학연구원 신약플랫폼기술팀 분자설계

The strategy for overcoming inhibition of human ether-a-go-go-related-gene (hERG) potassium channels to avoid drug induced cardiac arrhythmia has become an important factor during drug discovery. Recently, numerous in-silico methods have been developed either to meet with limited capacities for in vitro testing or to assess virtual compounds. In our work, we tried to establish the predictive QSAR models using Bayesian categorization and the recursive partitioning with various descriptors. The compounds that were measured in patch clamp settings using either HEK293 or Chinese hamster ovary (CHO) cells were taken from public domain literatures. The predictive power of our models were validated using in-house compounds.

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Molecular modeling for agonist selectivity at human 5-HT2 receptor subtypes

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G Protein-coupled receptors (GPCRs) is a tarket of more than half of drugs that are prescribed. Its selectivity is an important part of successful drug discovery and medicinal chemists need to design the compound differentiating among related receptor subtypes. The purpose of this work is to investigate the receptor-ligand interactions in the binding site of human 5-HT2A, 5-HT2B, and 5-HT2C receptor subtypes using molecular modeling techniques. With the absence of the crystal structure of human serotonin receptors, those 3D models were carried out by using homology modeling technique. Subsequently, protein-ligand docking was performed to generate distinct binding orientation of several agonists.

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In vitro and in vivo pharmacokinetic characterization of KR-66222 as a new candidate of type-2 diabetes agent

안성훈, 김민선, *송진숙, **이병회, ***안진희, ****배명애

*한국화학연구원 신약플랫폼기술팀 *충남대 약학대학 **한국화학연구원 신물질연구단 ***한국화학연구원 대사성질환연구팀 ****한국화학연구원 대사증후군치료제연구센타*

KR-66222 is a new candidate of type-2 diabetes agent developed by KRICT with the inhibition of dipeptidyl peptidase-4 (DPP-4), a major regulator of glucose metabolism in various tissues. Compared with sitagliptin (MK-0431), a recent DPP-4 inhibitor, KR-66222 showed higher in vitro activity of DPP-4 inhibition and similar in vivo activity of lowering glucose level. The purpose of this study was to characterize the pharmacokinetic profiles of KR-66222 in vitro and in vivo. Liver microsomal metabolic stability, cell permeability, and protein binding ratio of KR-66222 were studied. KR-66222 was stable (> 96 %) during 1 hr in both rat and human liver microsomal stability assay. However, the Papp value of KR-66222 across apical to basal in MDCK cell line was low (1.70 ± 0.13 x 10-6 cm/sec). Time-concentration profile of KR-66222 was showed in a multi-exponential manner in rats after intravenous and oral administration. The AUC value was 2.7 ± 0.74 (mg·hr/ml) and 0.12 ± 0.082 (mg·hr/ml) after intravenous and oral administration, respectively. The bioavailability was estimated 15.2 % after oral administration. This low F value of KR-66222 was mainly not affected by liver metabolism but by low intestinal absorption according to in vitro pharmacokinetic results. Even though KR-66222 had low bioavailability and may need further modification for higher bioavailability, the reason of similar in vivo DPP-4 inhibitory activity from KR-66222 might be higher activity of intestinal DPP-4 inhibition. This results suggests that low level of KR-66222 in systemic circulation can be enough for diabetes therapeutics.

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Molecular Docking Study for Glucokinase (GK) Activators

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Glucokinase (GK) is an emerging target for the treatment of diabetes mellitus as this is the major enzyme that catalyzes the phosphorylation of glucose in to glucose 6-phosphate. There are many synthetic activators are available for GK activation. But still there is a need for the development of potent GK activator. Furthermore, more structural and chemical feature information of GK activators was needed to study further rational activator design. In order to understand the binding mode of already known activators, molecular docking studies were performed with GK structure. In this study, key interacting residues were investigated based on comparative analysis of GK activator docked configurations.

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Pharmacophore Modeling and Virtual Screening for Novel Histone Deacetylase 8 Inhibitor Design

Sundarapandian, shalini, Sugunadevi Sakkiah, *이근우

*경상대 응용생명과학부 *경상대 생화학과*

Histone deacetylases are the enzymes that remove the acetyl groups from the N-terminal amino acids of histone proteins and thereby restrict the expression of various genes including cancer suppressor gene. Thus, the inhibition of this enzyme is emerging as new cancer therapeutics. A 3D QSAR pharmacophore model was generated using a training set of 20 diverse compounds. The best pharmacophore model with the correlation value of 0.935 was selected and validated using different methods and used further in database screening for novel virtual leads. Hits from the databases were subjected to molecular docking study using GOLD program. Based on the binding mode and interaction network at the active site three compounds were chosen and listed as potent virtual leads that could be utilized in designing novel potent HDAC 8 inhibitors as a new class of anti-cancer therapeutics.

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Molecular Dynamics Simulations Detailing the Importance of Bile Salts in Human Cholesterol Esterase

shalini, Sundarapandian, Sugunadevi Sakkiah, *이근우

*경상대 응용생명과학부 *경상대 생화학과*

Pancreatic cholesterol esterase (CEase) is a serine hydrolase that aids in the bile salt-dependent hydrolysis of dietary cholesteryl esters and thereby linked with the increased plasma cholesterol level. Inhibition of CEase can help treating various cholesterol related diseases such as coronary artery disease, obesity and diabetes. Molecular dynamics simulation (MDS) studies were performed to address the importance of proximal and distal bile salts for the enzymatic activity of human CEase. Co-ordinates of bile salts available from the crystal structure of bovine CEase was used to generate human CEase-bile salts complex. Results of MDS studies revealed the key points on the importance of the bile salts for the enzymatic activity of CEase. The overall effect upon the presence of each bile salt was observed. As a result, we found that both the bile salts are necessary for the enzymatic activity, but the effect of proximal bile salt was more influencing than the distal bile salt.

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Structure-based Virtual Screening for the Discovery of Novel Potent HSP90 Inhibitors

Sugunadevi Sakkiah, Sundarapandian, shalini, 메가나단, *이근우

*경상대 응용생명과학부 *경상대 생화학과*

Heat Shock Protein (HSP90) an ATP-dependent molecular chaperon which play a vital role in many signaling pathways. Hence the inhibition of HSP90 symbolizes a new target of antitumor therapy. A chemical feature-based modeling approaches has been applied to identify the crucial pharmacophore patterns based on the 3D crystal structures of five known inhibitors bound to human HSP90 (PDB IDs: 3BM9, 3HHU, 3BMY, 3FT8, 3EKR) using the software LigandScout and Discovery Studio V2.5. These five pharmacophore models where overlaid and removed the overlapped features and finally, 8 features pharmacophore was generated. This 8 features pharmacophore was split into two six features pharmacophore models, Hypo1 consist of 1 HBA, 1 HBD and 4 H groups and Hypo2 consist of 3 HBA, 1 HBD and 2 H groups. These two models were validated using the external test set eventually Hypo1 was selected as a best structure-based pharmacophore model for HSP90. The resultant pharmacophores were used for virtual screening of the databases like NCI, Maybridge and Chembridge. To refine the obtained outcomes from the virtual screening, ADMET and molecular docking were applied to sort out the screened molecules from the databases. As a result, finally we identified 23 compounds as the potent lead candidates for HSP90.

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Identify Novel Potential Inhibitors for PDE5 using Pharmacophore Modeling and Ligand-based Virtual Screening

메가나단, Sugunadevi Sakkiah, *이근우

*경상대 응용생명과학부 *경상대 생화학과*

Integrated computer-aided drug design technologies were utilized to generate pharamacophore modeling, database screening and docking methodologies for design of Phosphodiestrace5 (PDE5) inhibitors. The central role of PDE5 is hydrolyzes the cyclic guanidine monophosphate (cGMP) which leads male erectile dysfunction (MED). Three dimensional pharmacophore models were generated using HypoGen algorithm implemented in Discovery Studio v2.1. The pharmacophore model, Hypo1, characterized one hydrogen bond acceptor (HBA), one hydrogen bond acceptor lipid (HBAL), one hydrophobic (HY), and one ring aromatic (RA) feature. The high cost difference (110.599), good correlation coefficient (0.94) and low root mean square deviation (1.53) were suggested that Hypo1 was highly predictive pharmacophore model. Further, Hypo1 model has been validated by Fischer's randomization method, wide range of test molecules, and decoy set. The validated Hypo1 was then used as 3D search query to perform a virtual screening. Subsequently, the hit compounds were subjected to filtering by Lipinski's rule, ADMET and molecular docking to refine the retrieve hits. As a result, the optimized three dimensional pharmacophore model was obtained and we think that this model will act as valuable tool for the virtual screening to identify new potential leads of PDE5.

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A Simple and High-Throughput Method for Assessing Druggability of Small molecules

Eun Jeong Cho, *이주운

*The Texas Institute for Drug and Diagnostic Development, The University of Texas at Austin, Austin, TX 78712 *충주대 교양학부 - 화학*

We present a simple, inexpensive, robust, and high throughput method for early stage duggability assessment. The method utilizes fluorescent probe, ethidium bromide (EB), in which its inherent fluorescence intensity increases upon binding to nucleic acids. The fluorescence signal diminution when EB is displaced by small competing chemicals provides a quantitative tool to compare, or rank, non-specific nucleic acid binding and is therefore directly applicable to evaluate toxicity of chemical compounds. Full details of assay optimization, miniaturization, automation, and validation and results of screening 446 chemical compounds from NIH clinical collection will be discussed. The result demonstrated that comparative biological analysis of non-specific binging affinities allows us to quickly examine druggability of small molecules and prioritization of compounds from commercial or house-produced libraries at very early drug development stage.

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Active Ester-Functionalized Polythiophene for Conducting Scaffolds in Tissue Engineering

정의덕, *이주운

*한국기초과학지원연구원 하이테크부품소재연구지원센터 *충주대 교양학부 - 화학*

Recent advances in bioengineering have led to increased interest in the nature of surface and interfacial phenomena of conductive biomaterials. Here, we present the synthesis and physicochemical characterization of conductive poly(3´-carboxyl-5,2´:5´,2˝-terthiophene) (PThCOOH). The carboxylic acid surface of PThCOOH is chemically conjugated with the cell- recognizable Arg-Gly-Asp (RGD) motif. Normal human dermal fibroblast cells cultured on RGD-modified PThCOOH demonstrate significantly improved attachment and spreading. Further studies are currently underway to develop functionalized polythiophene composites as bioactive conducting scaffolds for specific tissue engineering purposes.

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Preparation and Characterization of Adenosine Functionalized Multi-walled Carbon Nanotubes with Gold Nanoparticles

PHAM TUAN ANH, 정연태

부경대 이미지시스템공학과

Covalent functionalization of multi-walled carbon nanotubes (MWNTs) has emerged as an important method to obtain the water-dispersible multi-walled carbon nanotubes, and to introduce noble metal nanoparticles to the surface of nanotubes for the construction of hybrid nanostructures. In this study, water-dispersible MWNTs were successfully prepared by chemical grafting adenosine onto the surface of nanotubes via esterification or amidation reaction. Then, the anchoring gold nanoparticles on the nanotubes was carried out by a new strategy via boroester linkages, which were formed by reaction of free hydroxyl groups between adenosine-functionalized MWNTs and boronic acid-functionalized gold nanoparticles. Morphological and structural characteristics of hybrid nanostructures were characterized using various techniques including FT-IR, UV-vis, HR-TEM, FE-SEM and XPS spectra.

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Synthesis of Gold Nanostructures Using a Detergent and Their Catalytic Activity

Thathan Premkumar, 김성호, *K. E. Geckeler

*광주과학기술원 신소재공학과 *광주과학기술원 신소재공학과,나노바이오전자재료공학과*

A simple method for the synthesis of gold nanostructure via the reaction of an aqueous solution of a gold salt, the potassium tetrachloroaurate(III), with a detergent at room temperature was developed. The as-prepared gold nanoparticles were characterized by UV-vis, UV-vis-NIR spectroscopy, transmission electron microscopy, and atomic force microscopy. It was found that the shape of the gold nanostructures can be manipulated by changing the reaction conditions such as the concentration of the reactants as well as the temperature. Further, the gold nanostructures showed a catalytic activity for the reduction reaction of 4-nitrophenol in the presence of sodium borohydride, which has been monitored by UV-vis spectroscopy. This method is facile and employs gentle reaction conditions in contrast to the conventional techniques using polymers or surfactants and harsh reductants.

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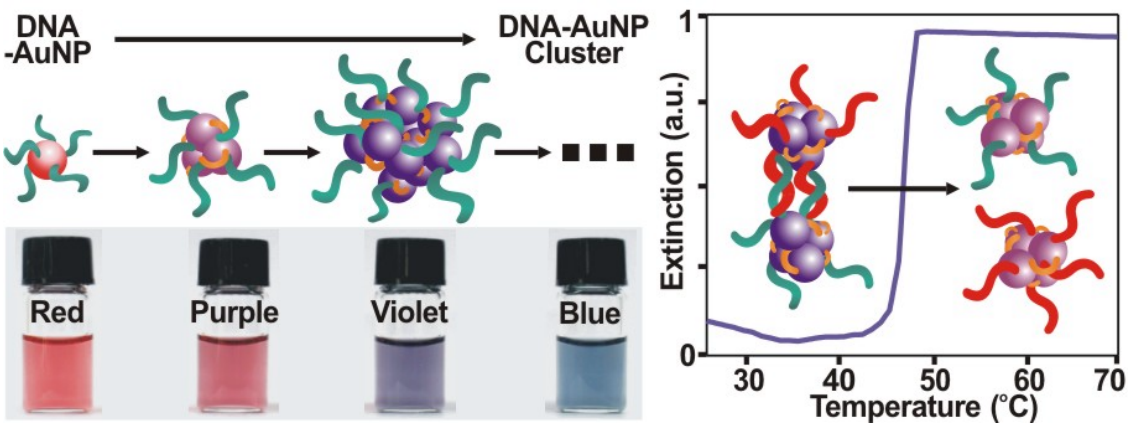
Synthesis and Thermally Reversible Assembly of DNA-Gold Nanoparticle Cluster Conjugates

김지영, 이재승

고려대 신소재공학부

We describe the facile synthesis of stable gold nanoparticle clusters densely functionalized with DNA (DNA-AuNP clusters) using dithiothreitol and monothiol DNA and their thermally reversible assembly properties. The size of the clusters exhibits a very narrow distribution and can be easily controlled by adjusting the stoichiometry of dithiothreitol and DNA, leading to a variety of colors due to the surface plasmon resonance of the AuNP clusters. Importantly, the DNA-AuNP clusters exhibit highly cooperative melting properties with distinctive and diverse color changes depending on their size. The selective and sensitive colorimetric detection of target sequences is demonstrated based upon the unique properties of the DNA-AuNP clusters.



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Covalent polymer functionalization of Graphene nanosheets with conjugated polymers: Novel Hybrid materials

NANJUNDAN ASHOK KUMAR, 정연태

부경대 이미지시스템공학과

Recent years have witnessed great advances in the functionalization chemistries of carbon based nanomaterials, which is a rapidly and continuously growing. Graphene sheets are now considered to be a valuable synthon in nano materials chemistry due to its unexplored properties. There are a number of polymers having importance and playing a significant role in the semiconductor industry which are yet to be investigated of its role with graphene. Among them conducting and conjugated polymers are an important class of polymers which has great prospects with semiconductor industries and molecular electronics. Here, we report the covalent functionalization strategy to graft the conjugated polymer propylene dioxythiophene with graphite oxide as novel nanocomposites. FTIR spectroscopy was employed to characterize the change in surface functionalities which revealed that the PProDOT was covalently grafted to the MWNTs while TGA was used to study the weight gain. The morphology micrographs of the grafted PProDOT on GNS as evidenced by TEM showed apparent effect on the structure of the sheets as a result of surface modification. Our experimental results indicate that the complex exhibited improved thermal stability. Due to the wide role and importance of PProDOT in electrochromic devices, these hybrids are expected to have practical and great potential applications for high performance devices.

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Surface functionalization of multiwalled carbon nanotubes with ammonium based ionic liquids

NANJUNDAN ASHOK KUMAR, 정연태

부경대 이미지시스템공학과

Carbon based nanomaterials have gained intense attention from both academics and industries due to their extraordinary properties. Their use for fabrication of reinforced polymer composites, field-emission displays, hydrogen storage are being envisaged and investigated extensively. The present study reports the functionalization of multiwalled carbon nanotubes (MWNTs) with novel ammonium based ionic liquids. Acid oxidized MWNTs were first acylated using thionyl chloride and further functionalized with choline dihydrogen phosphate, a novel materials. The resulting ionic liquid functionalized act as dispersing agents to well disperse CNTs in organic solvents. The covalent route reported here to functionalize MWNTs with ionic liquid through chemical grafting technique has many advantages. The nanocomposites were well characterized with the necessary analytical techniques namely field emission scanning electron microscopy (FE-SEM) and high resolution transmission electron microscopy (HR-TEM). The changes in surface functional groups were analyzed using X-Ray photoemission spectroscopy (XPS) and attenuated total reflectance infrared spectroscopy (ATR-IR). The microscopic images revealed that the covalent functionalization procedure was effective and provided a firm coating of the soft material on nanotube side-walls. The coating of CNTs with the novel ionic liquid enhanced the thermal properties of the complex when compared to that of pristine nanotubes.

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TiO_2 photocatalysts modified with uniform gold nanoparticles

이명순, 이동일

연세대 화학과

The deposition of noble metal nanoparticles on semiconductor surface can increase the efficiency of photocatalytic reaction due to their role as a reservoir for photogenerated electrons. Although they can promote charge carrier separation and interfacial charge-transfer processes in noble metal nanoparticles/semiconductor composite system, there is still unsettled problem concerning the control of size, shape and electron transfer of noble metal deposits. In this presentation, we have investigated a new strategy to prepare well-defined nanoparticle photocatalysts using monolayer-protected gold clusters (MPCs). TiO_2 modified with uniform Au MPCs via a bifuntional linker, glutathione, exhibited high photostability and enhanced photocatalytic activity for the photoreductive degradation of a model dye, Uniblue A (UBA), under UV illumination. While there is little enhancement in photocatalytic activity found for TiO_2 modified with Au MPCs, the activity significantly increases upon thermal activation of AuMPC-TiO_2 assemblies. TEM images showed that the Au MPCs core size was maintained after anchoring to TiO_2 and thermal activation of the AuMPCs-TiO_2 assembles. In addition, the effects of the linker between TiO_2 and the gold core on the charge separation and photocatalytic activity will be discussed.

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High resolution patterning method by using LIquid-mediated Nano transfer direct printing

당정미, 조보람, 성명모

한양대 화학과

We report a new direct printing method, called Liquid-mediated nano transfer direct printing that uses a polar liquid-mediated transfer process. Liquid-mediated nano transfer direct printing is based on the direct transfer of various materials from a stamp to a substrate via a liquid- bridge between the stamp and the substrate. This procedure can be adopted in automated printing machines that generate various material patterns with a wide range of feature sizes (as small as 60 nm) on diverse substrates. The patterns have been investigated by scanning electron microscopy(SEM).

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Three-Dimensional Nanofabrication with Nanotransfer Printing using Atomic Layer Deposition

김수환, 성명모

한양대 화학과

We report a new patterning technique of inorganic materials by using thin-film transfer printing (TFTP) with atomic layer deposition. This method consists of the atomic layer deposition (ALD) of inorganic thin film and a nanotransfer printing (nTP) that is based on a water-mediated transfer process. In the TFTP method, the Al_2O_3 ALD growth occurs on FTS-coated PDMS stamp without specific chemical species, such as hydroxyl group. The CF_3-terminated alkylsiloxane monolayer, which is coated on PDMS stamp, provides a weak adhesion between the deposited Al_2O_3 and stamp, and promotes the easy and complete release of Al_2O_3 film from the stamp. And also, the water layer serves as an adhesion layer to provide good conformal contact and form strong covalent bonding between the Al_2O_3 layer and Si substrate. Thus, the TFTP technique is potentially useful for making nanochannels of various inorganic materials.

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Fabrication of Solution Processed TIPS-Pentacene Thin-Film Transistor by Using Nanotransfer Molding

황재권, 오현석, 성명모

한양대 화학과

We report a new direct printing method, called liquid-mediated nanotransfer moldig (LB-nTM), that uses a polar liquid-mediated transfer process. LB-nTM is based on the direct transfer of various materials from a stamp to a substrate via a liquid-bridgebetween the stamp and the substrate. This procedure can be adopted in automated printing machines that generate various material patterns with a wide range of featuresizes (as small as 60 nm) on diverse substrates. To demonstrate its usefulness, the LB-nTM method was applied to prepare TIPS-pentacene transistors. A high field-effect mobility of 0.02 cm^2 V^{-1} s^{-1} was achieved in the saturation regime of VD -40V along with an on/off current ratio of $\approx 10^5$ and a threshold voltage of -5V.

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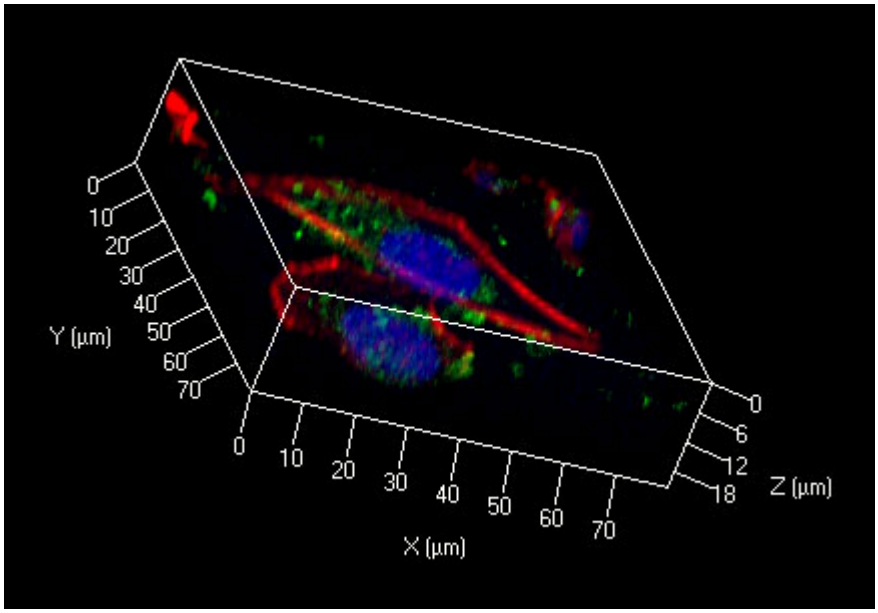
Mesoporous Hollow Silica Capsules with a Large Pore Opening: Intracellular Delivery of Membrane-Impermeable Proteins, Molecules and Ions

허성, 임지선, *이기원, 황용경, **김성진, *권혁만

*한국외국어대 화학과 *한국외국어대 생명공학과 **이화여대 화학과*

Mesoporous rods and spheres with suitable pore dimensions and organic functionalities have been extensively prepared and employed in a variety of biological applications such as bioimaging and delivery. Both shape and organic functionality on the surface of mesoporous silica nanoparticles (MSNs) played an important role in the efficacy of small drug molecule delivery into HeLa cells. Here we report our new preparation method of hollow mesoporous silica capsules with a large pore opening. Pure siliceous capsule, carboxy-capsule, and amino-capsule were successfully prepared and characterized by gas sorption, TEM, SEM, and PXRD. Due to the large pore opening, the mesoporous capsules are suited for the intracellular delivery of proteins as well as various cell membrane-impermeable molecules and ions. The CLSM result, TEM and FACS data clearly support their efficient transport into HeLa cells. Compared with pure siliceous capsule, the amino-capsule exhibited almost no cytotoxicity for a prolonged incubation period supported by WST-1 assay tests and cell proliferation experiments conducted for 96 h. It was also possible to functionalize the surface of carboxy-capsule with other amine-containing molecules for further applications. For example, 5-aminofluorescein could be successfully attached on the surface of carboxy-capsule through a simple amidation. Green fluorescent protein (GFP) delivery will also be demonstrated.



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Synthesis and photovoltaic properties of Dye-sensitized solar cells using newly synthesized organic Dyes

조주열, 이선영, 황도훈

금오공과대 응용화학과

Dye-sensitized solar cells (DSSCs) have developed rapidly by many research groups because of their various advantages, such as high efficiency and low-cost devices for solar cells. Mainly DSSCs can divide with two parts, inorganic dyes and organic dyes. Inorganic dyes have been studied a lot and it gave also good results. For example Ru-polypyridyl-complex dyes, such as cis-dithiocy-anato bis(4,4`-dicarboxy-2,2`-bipyridine)ruthenium(II) (called N3 dye) can produce solar energy-to electricity conversion efficiency (è) of up to 11% under AM 1.5 G irradiation. Besides N3 dyes, metal-free organic dyes have been utilized in DSSCs because of their wide variety of the structures, facile modification, and high molar absorption coefficient. In this work we have designed and synthesized simple metal-free organic dyes for DSSCs and also have identified their photovoltaic properties.

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Synthesis and Characterization of New Two-dimensional Chromiun Thiophosphates, $CsCrP_2S_7$

박소정, *윤호섭

*아주대 응용화학 *아주대 화학과*

The new quaternary Thiophosphate, $CsCrP_2S_7$ has been synthesized through the reaction of elements with alkali metal halide and structurally characterized by single crystal X-ray diffraction techniques. The title compound crystallizes in the space group C_2^3-C2 of the monoclinic system in a cell of a=8.5801(5)Å, b=9.5345(6)Å, c=6.7449(6), β=97.530(3), V=547.02(7)$Å^3$. The compound is comprised of two-dimensional $(_\infty^2)[CrP_2S_7]^-$ layers separated from one other by the Cs^+ cation through the ionic interactions. The layers are built up from the basic repeating unit $(_\infty^2)[Cr(PS_4)_2S_2^{2-}]$, which is composed of the bitetrahedral thiophosphate $[P_2S_7^{4-}]$ anions sharing edges and corners with $[CrS_6]$ octahedra. The Cs^+ ion is coordinated by eight sulfur atoms, four from each the two $[CrP_2S_7]$ adjacent layers. The classical charge of the compounds can be represented by $[Cs^+][Cr^{3+}][P^{5+}]_2[S^{2-}]_7$. In this paper, the magnetic properties in the 5-300K temperature range will be discussed along with the other related quaternary thiophosphates in different oxidation state of chromium.

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투명도전성 박막제조용 인듐저감 조성물 연구

박종일

포항산업과학연구원 원천소재연구본부

FPD 용 투명 도전막의 제조에 핵심소재로 사용되고 있는 ITO 타켓재 물질에서 인듐 소재의 자원고갈로 인해 대체 또는 저감 기술이 요구되고 있다. 본 연구에서는 인듐 사용량 저감을 위한 인듐-갈륨-아연 산화물의 복합체의 조성물에 대한 연구를 수행하였다. In_2O_3, Ga_2O_3, 그리고 ZnO 를 주성분으로 하는 금속산화물 복합체 제조하고 및 이를 타겟으로 가공하여 스퍼터링하여 투명도전성 박막을 제조하였다. 인듐, 갈륨, 아연 및 산소로 이루어진 (In+Ga)/(In+Ga+Zn)의 원자비가 15~85 at. %의 비율에서 투과율 90% 이상, 100 옴/squre 이하의 표면 저항값을 가진 조성을 얻을수 있었다.

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Synthesis and Characterizations of a New QuaternaryTitanium Thiophosphates, $Cs_3Ti_3(P_4S_{13})(PS_4)_3$

김경희, *윤호섭

*아주대 에너지시스템학부 *아주대 화학과*

New quaternary titanium thiophosphates, $Cs_3Ti_3(P_4S_{13})(PS_4)_3$ has been synthesized with the reactive halide flux and structurally characterized by single-crystal X-ray diffraction techniques. The compound is isostructural with $Rb_3Ti_3(P_4S_{13})(PS_4)_3$. The structure of the compound is constructed by the interconnection of octahedral $[TiS_6]$ units and two types of thiophosphate ligands, $[PS_4]^{3-}$ and $[P_4S_{13}]^{6-}$ anions. The $[P_4S_{13}]^{6-}$ anion is composed of three $[PS_4]$ tetrahedra sharing corners with one $[PS_4]$ group in the center of the star-like anion. The $[TiS_6]$ octahedra share two edges with the $[PS_4]^{3-}$ tetrahedra in the sequence of –P-Ti-P-Ti-P- yielding an infinite helical chain. Two different type of helical chains are connected to form two different helical tunnels along the c-axis. As a guest ion, Cs^+ cation intercalated into the empty channel with ionic interaction to stabilize the three-dimensional structure through electrostatic ionic interactions. The classical charge balance of the title compound can be described as $[Cs^+]_3[Ti^{4+}]_3[PS_4^{3-}]_3[P_4S_{13}^{6-}]$.

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MgO protective layer using nanopowders prepared by RF plasma

박종일

포항산업과학연구원 원천소재 연구본부

MgO thin films and nonapowders are widely used as dielectric layers of plasma display panel (PDP). Secondary electron emission coefficient of the thin films is a key factor for reduction of electric consumption of PDP. In this study, nanopowders of MgO are synthesized by radio frequency (RF) plasma technique. Their structure, morphology and particle size distributions are determined by XRD and TEM analysis. By using nanopowders of MgO, the deposited films showed good secondary electron emission coefficient values than conventional MgO films.

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Development of New Organic Solar Cell Material for Environment-friendly Green Energy

권준호, 안지영, 장한메, 최솔지, *김윤희, *이민정, 박진희

*경남과학고 *경상대 화학과*

좁은 밴드갭, 높은 개방전압, 높은 단락전류를 가져 고효율 특성을 나타낼 것으로 예상되는 유기태양전지용 고분자를 설계합성하고 물성을 평가하였다. 고분자는 Suzuki 반응 등 잘 알려진 유기반응을 통해 합성하였으며, NMR 과 FT-IR 로서 확인하였다. 분자량에 따른 용해도의 차이를 이용하여 분자량이 다른 고분자를 분리하였다. 고분자의 열분석, 자외선-가시광선 스펙트럼 및 전기화학 분석으로 고분자가 좁은 밴드갭과 넓은 영역의 광흡수 특성, 5.4 eV 의 깊은 HOMO 값, 높은 열안정성을 가지는 것으로 확인되었으며 분자량에 따른 고분자의 특성차이에 대한 연구도 같이 수행하였다. 얻어진 고분자를 PC70BM 과 혼합하여 태양전지 소자를 제작한 결과를 발표하고자한다.

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First examples of new blue-violet emitters based on indenopyrazine core system for OLEDs : effects of the substitution positions of m-terphenyl side group on their optical and electroluminescent properties

박영일, *이지훈, **정동현, 박종욱

*가톨릭대 화학과 *충주대 나노고분자공학과 **(주)인실리코텍*

A promising class of blue-violet emitters based on a new functional core, the indenopyrazine group, has successfully been synthesized for the first time by substitution with bulky m-terphenyl side groups in the ortho, meta, or para positions. There are larger blueshifts in the UV-visible and PL spectra of the synthesized ortho- and para- substituted derivatives than in those of the meta- substituted derivative. Molecular calculations verified that these differences are due to the variation in the π-conjugation length of the derivatives with the position at which the side group is attached to the indenopyrazine core. When the synthesized compounds were used as emitting layers in non-doped OLED devices, a related trend was observed in their optical properties. In particular, the OLED containing the para-substituted derivative was found to exhibit excellent characteristics, with maximum EL emission at 423 nm, pure violet emission with CIE coordinates (0.173, 0.063), and an external quantum efficiency of 1.88%.

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Photocatalytic behavior of a heterojunction between tungsten doped SnO_2 and TiO_2 under visible light Irradiation

Rawal Sher Bahadur, 김학진, 김용주, 이완인

인하대 화학과

Tungsten-doped tin oxide ($W_xSn_{1-x}O_2$, x=0.05) was prepared by co-precipitation of $SnCl_4.5H_2O$ & WCl_4 with post annealing & characterized by XRD, SEM & TEM. The optimum doping level of tungsten was found to be 5% & with increasing doping level, segregation of tungsten on the surface of SnO_2 appears which was confirmed by XRD. $W_xSn_{1-x}O_2/TiO_2$, a heterojunction structure between tungsten doped tin oxide and TiO_2, was prepared by covering the surface of the 50 nm-sized $W_xSn_{1-x}O_2$ particles with TiO_2 by sol-gel method. It was found that $W_xSn_{1-x}O_2$ shows a profound absorption over the visible range in comparison to pure SnO_2 and its valence band (VB) is located lower than that of TiO_2. As a result, under visible light irradiation ($\lambda \geq 420$ nm), $W_xSn_{1-x}O_2$ showed a notably high photocatalytic activity in removal of gaseous 2-propanol and evolution of CO_2. The high photocatalytic efficiency of the $W_xSn_{1-x}O_2/TiO_2$ under visible light irradiation was therefore deduced to be caused by the hole transfer between the VB of $Sb_xSn_{1-x}O_2$ and TiO_2.

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Efficient organic sensitizers for use in Dye-Sensitized Solar Cells (DSSCs)

강영진, *고재중, **김진호, **이은지, **정나래

*강원대 과학교육과 *고려대 소재화학과 **강원대 화학과*

In designing metal-free sensitizer, it is important to escape from π-π stacking of adsorbent sensitizer at the TiO_2 surface. Better morphological stability of the amorphous phase is often noted for metal-free sensitizer. In addition, strongly conjugated sensitizers should have wide absorption range in visible region which leads to wide light harvesting properties and consequently ensure high electron-transfer rate. The control and modification of spacer group in the design of organic sensitizer have attracted attention since photo-current efficiency in DSSCs may depend on the nature of sensitizer, and spacer as well as donor segments in sensitizers play a key role in determination of efficiency. The effect of spacer unit in the presence or lack of bulky group on DSSCs performance was systematically investigated.

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Formation of efficient dye-sensitized electrodes by low-temperature process employing nanoporous spherical TiO_2 structures

장세희, 유인경, 문정훈, 이완인

인하대 화학과

Sub-micrometer-sized TiO_2 spheres with an ultra-high surface area were successfully applied to the low-temperature process of dye-sensitized electrodes. TiO_2 sphere induces significantly increased surface area, improved electron transport property, and higher quantum efficiency in the long wavelength region. As a result, The photovoltaic conversion efficiency was enhanced from 4.4% to 6.3%.

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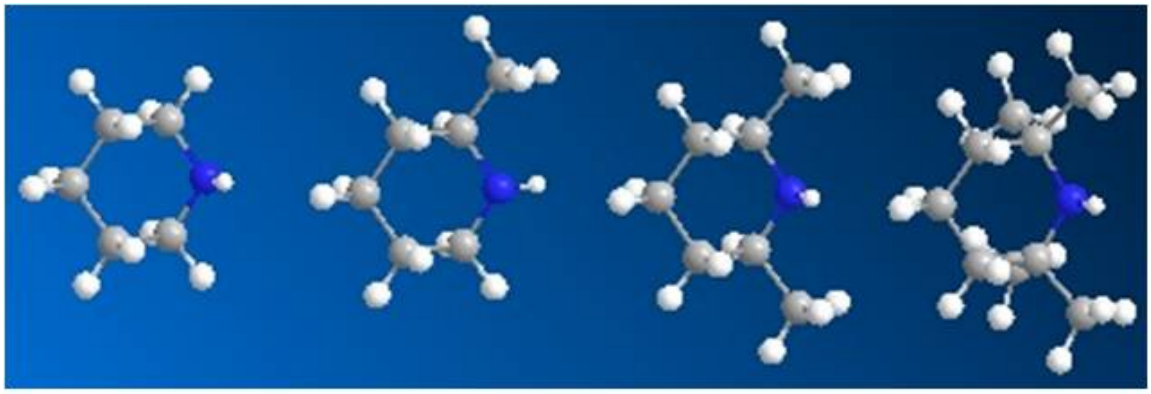
Effect of structure directing agent containing piperidine moiety on structure of aluminaphosphate : Synthesis and structural determination of powder diffraction

주빛나, *신혜선, 장익준, *조성준

*전남대 신화학소재공학과 *전남대 응용화학공학부*

Aluminophosphate (AlPO) has been synthesized hydrothermally with the variation of moiety of structure directing agent (SDA) as shown in Figure 1. The structure of the obtained AlPO was AlPO-5 (AFI) with the parent SDA, piperidine (PI). Increasing the number of methyl group on PI resulted in the formation of new AlPO structure containing SAS framework when 2,2,6,6,-tetramethylpiperidine (TMPI) was used as SDA. The obtained crystal structure with Rietveld refinement of powder diffraction (R_p=0.078 and R_{wp}=0.078) was *P 4/nnc* with a=1.4235 nm and c=1.01008 nm, which was similar to that of STA-6. Thermal decomposition of the obtained AlPO sample induced partial structural change but the sample contained appreciable surface area and pore volume, 140 m^2g^{-1} and 0.073 ccg^{-1}, respectively.



PI MPI DMPI TMPI

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Surface-Enhanced Raman Scattering of Graphene: Dependence on Excitation Wavelength and Comparison of Single-Layer and Few-Layer Graphene

이지숙, *심상덕, **김봉수, 신현석

*울산과학기술대 에너지공학부 *삼성전기(주) 중앙연구소 분석그룹 **KAIST 화학과*

Surface-enhanced Raman scattering (SERS) of graphene has been studied by depositing Au nanoparticles on graphene using thermal evaporation. An optimum condition for SERS measurement of graphene was first investigated by changing density of evaporated Au nanoparticles and excitation wavelength. When aggregated Au nanoparticles were formed on single-layer graphene and 633 nm was used as an excitation wavelength, SERS enhancement factor was maximum 120. While no band was observed in normal Raman spectrum before evaporation of Au using 785 nm, unlike 532 and 633 nm, only G band was significantly enhanced in SERS spectrum after evaporation of Au. Thus, SERS enhancement factor has not been determined when 785 nm was used as an excitation wavelength. Also, differences between single-layer and few-layer graphene were investigated by comparing their SERS images and spectra. The SERS enhancement factor in single-layer graphene was much larger than that in few-layer graphene and in single-layer graphene the SERS enhancement factor for the G band was larger than that for the 2D band. Moreover, the D band was observed in the SERS spectrum which has not appeared in a normal Raman spectrum before evaporation of Au. Appearance of the D band is not due to Au-induced defect but due to large enhancement of the D band from very small amount of defects on graphene.

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Determination of Solubility Parameter of Carbon Nanotubes by Inverse Gas Chromatography

임형준, 박종래

서울대 재료공학부

The determination of solubility parameters by inverse gas chromate graphy (IGC) for as-produced and surface functionalized Carbon Nanotubes (CNTs) is discussed.To solve the aggregation problem of CNTs, numerous modification methods have been introduced. However, there is still no systematic study about the dispersion of CNTs. Therefore, to overcome the limitations, the knowledge of the solubility parameter of carbon nanotubes for different CNTs is important for predicting the dispersion behavior of CNTs in solutions and composites.Inverse gas chromatography method is widely used for the characterization of polymers and surfactants that are capable to offer adsorption thermodynamics parameters, dispersive surface tension and solubility parameter. However there are only limited reports about CNTs, especially the surface functionalized ones, because of thermal degradation problems of functional groups in working condition of IGC or inaccurate retention parameters due to the surface characteristics of CNTs.Thus in this research, we found adequate working condition of adjusting IGC to determine the solubility parameters of CNTs. Then under this condition, the solubility parameters of CNTs were found by carrying out IGC. This study confirmed that the IGC method can be successfully applied to determine unknown solubility parameters of various CNTs. Also we found small modification of functional group can greatly affect solubility parameters of CNTs. The determined solubility parameters are well fit with the pre-reported dispersion stability of CNTs. Therefore it is expected that the results obtained in this work would assist in providing a guideline in finding the solubility of CNTs.

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Synthesis and Surface-Enhanced Raman Scattering of Triangular Gold and Noble Metal Core-Shell Nanoprisms

Dickson Joseph, *K. E. Geckeler

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Surface-enhanced Raman scattering (SERS) integrates high levels of sensitivity with spectroscopic precision, and thus, has tremendous potential for chemical and biomolecular sensing. In this regard gold-silver core-shell triangular nanoprisms (TNs) have been prepared from gold nanoprisms by using a two-step method. Firstly, triangular gold nanoprisms were prepared by reducing potassium tetrachloroaurate in an alkaline solution of cyclodextrin in the presence of Tween 80. Subsequently, the gold-silver core-shell TNs were synthesized from silver and ascorbate ions using the Au TNs as the seeds in the presence of poly(1-vinyl-2-pyrrolidone). In addition to the Au-Ag bimetallic TNs, gold-palladium and gold-platinum TNs were also synthesized using the same procedure. The bimetallic Au-Ag core-shell triangular nanoprisms containing a silver shell provide an elegant and powerful SERS-active substrate when compared to the corresponding monometallic Au nanoprisms. The enhanced surface Raman scattering signals were attributed to the local field enhancement in the core-shell structure.

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The Regular Arrays of TiO_2 Nanotubes Photoelectrodes with CdSe/CdS layers deposited inside for the Photolysis of Water using UV and Visible Lights of a solar emission

신연미, 이성훈

서울대 화학부

Titanium dioxide (TiO_2) is one of the most important materials extensively investigated for use in water photoelectrolysis, due to the proper band edge position and photostability. However, the wide bandgap (3.0-3.2 eV) of TiO_2 limits its photoresponse in the UV region. Recently, we reported the fabrication of highly ordered TiO_2 nanotube arrays with a high aspect ratio through a two-step anodizing process using electropolished flat titanium.Here, we report the regular arrays of TiO_2 nanotubes photoelectrodes with CdSe/CdS layers deposited inside and their application as a photoanode for the photolysis of water. CdS and CdSe nanoparticles are deposited onto the inside of TiO_2 nanotubes using a chemical bath deposition (CBD) process to extend the photocatalytic activity into the visible light region. Further these electrodes are utilized for the production of hydrogen resulting from the split of water in a photoelctrochemical cell under a simulated AM 1.5 illumination.

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Thermodynamic and Electrical Characteritics of $NdBaCo_2O_{5+\delta}$ in a Reducing Environment

유선영, *신지영, 김건태

*울산과학기술대 친환경에너지공학부 *동의대 기계공학과*

Solid oxide fuel cell is the device that converts the chemical energy in fuel to the electrical energy directly with high efficiency. Cation ordered perovskite-related oxides, $NdBaCo_2O_{5+\delta}$(NBCO), is known as one of the best cathode materials for intermediate-temperature solid oxide fuel cell(IT-SOFC) because of its rapid oxygen diffusion and surface exchange kinetics and high electrical conductivity. The purpose of redox characteristics is to identify the above properties of the $NdBaCo_2O_{5+\delta}$ as a candidate for IT-SOFC cathode material with the appropriate experimental techniques, such as XRD, 4-probe conductivity, and coulometric titration(CT). Thermodynamic redox characteristics including oxidation enthalpies and entropies were studied by the CT. The isotherms were obtained at 650, 700 and 750℃ over a broad range of pO_2. Oxygen non-stoichiometry has shown that higher temperature lead more reduction of the NBCO at the same pO_2 region, involving that its decomposition at 750℃ occurred near the pO_2 of 10-5atm, but it was not detected at 650℃ within the operational range of the SOFC cathode (pO_2 of 10-5atm). Therefore, the NBCO may not be suitable for the cathode of SOFC above operating temperature of 750℃ due to the decomposition. The oxidation enthalpies increased quite a lot even with small change in the reduction state, which were -338.2 kJ/mol-O_2 and -506.0 kJ/mol-O_2 at δ=0.412 and 0.392, respectively. Also the oxidation entropies were determined as -305.3 J/mol-O_2/K and -469.0 J/mol-O_2/K at δ=0.412 and 0.392, respectively. The electrical conductivities were measured by 4-probe method over a broad range of pO_2. This material indicated sufficiently high conductivities for IT-SOFC cathode application.

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The Formation of Hybrid Organic-Inorganic Zincone Thin Films by Molecular Layer Deposition through three sequential reaction steps

조성권, 이성훈

서울대 화학부

Hybrid organic-inorganic thin films were grown by molecular layer deposition. Molecular layer deposition (MLD) similar to atomic layer deposition (ALD) is a sequential, self-terminating growth process. In the growth of hybrid organic-inorganic thin films, we used diethyl zinc(DEZ), ethanolamine(EN), and vinylene carbonate(VC) as reactants. An MLD consists of three sequential steps: in the first step, ethyl zinc is pulsed onto a substrate and then its remnant is removed by a purging Ar, in the second step, ethanolamine (EN) is pulsed onto the substrate and then is removed by a purging Ar, in the third step, vinylene carbonate (VC) as a ring-opening reactant is pulsed onto the substrate and later is removed by a purging Ar. As like alucone polymers of the form $(\text{-O-Al-O-R-})_n$, the resulting hybrid organic-inorganic thin film is an Zincone with the form $(\text{-Zn-OCH}_2\text{CH}_2\text{NH-C(O)OCHCHO-})_n$. We characterized the composition, thickness, and structural image of the Zircone thin film using ex-situ FTIR spectroscopy, ellipsometry, and transmission electron microscopy, respectively. These results demonstrate that an MLD is an ideal method to fabricate hybrid organic-inorganic thin films that can be useful in various flexible electronic devices.

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Manganese oxide에 미량의 금속원소 첨가가 spinel 구조 형성에 미치는 영향

김양수, *양경모, *이우람, *김정준, *류현주, *송혜정

*한국기초과학지원연구원 순천센터 *전남대 화학과*

나노물질를 여과하기 위한 분리기술은 꾸준히 발전해왔다. 나노물질을 여과하기 위한 물질 중의 하나인 망간산화물은 좋은 양이온 교환능력과, 분자흡수능력을 보여 나노이온 분자의 여과뿐만 아니라 촉매로의 가능성이 높다고 알려져 있다. 본 연구에서는 나노물질의 여과에 사용되는 흡착제의 합성을 기존의 수열방법과는 달리 고상반응법을 통해 제조하였다. 이 반응은 기존의 액상반응법이 아닌, 대량생산이 용이한 고체상태의 시료로써 반응시키기 때문에 주목할 만한 의미가 있다. 또한 현재까지의 연구에서는 o-$Li_{1+x}Mn_{1-x}O_2$ 의 경우 낮은 결정성으로 인해 새로운 구조를 갖는 $Li_{1.6}Mn_{1.6}O_4$ 로 상변화가 일어나며 이 화합물은 다량의 이온 교환능력을 가진다는 것을 밝혀졌는데 본 연구에서는 기존에 $Li_{1.1}Mn_{0.9}O_2$ 에 새로운 원소를 첨가한 것에 대해 그 결과를 보고 새로운 흡착성능을 가진 리튬이온 흡착제를 제조, 분석하고자 한다.

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Photochemistry of dye sensitized solar cell based on N-doped TiO2 hollow nanospheres

임정섭, *조형준, **정동운

*원광대 생명나노화학과 *원광대 생명나노화학부 **원광대 화학과*

질소가 치환된 속이 빈 구형의 TiO2 나노입자를 합성하고 이를 이용하여 염료감응형 태양전지를 제조하였다. TiO2 입자를 일반적인 양극물질로 사용했을 경우에 비하여 scattering layer 로 사용했을 경우 태양전지의 효율이 증가하였다.

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Photocatalytic property of N-doped TiO_2 hollow nanospheres

조형준, *임정섭, **정동운

*원광대 생명나노화학부 *원광대 생명나노화학과 **원광대 화학과*

질소가 치환된 속이 빈 구형의 TiO_2 나노입자를 제조하였다. 입자의 제조를 위하여 Inorganic template 를 사용하였다. 질소 치환된 속이 빈 구형의 TiO_2 입자는 일반적인 구형의 입자에 비하여 가시광선 영역에서 광촉매 활성이 우수하였다.

THE KOREAN CHEMICAL SOCIETY

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CdSe Gradient Shell Nanocrystals : Synthesis and Characterization

김경남, *한창수, **정소희

*한국기계연구원 나노역학실험실 *한국기계연구원 나노공정장비센터 **한국기계연구원 나노기계연구본부*

Semiconductor nanocrystal quantum dots (NQDs) are near-ideal fluorophores for biological applications ranging from single-molecule fluorescence spectroscopy/imaging to biosensor platforms. NQDs are characterized by broadband absorption, narrow and tunable emission, exceptional brightness, and resistance to photobleaching. They are sufficiently small (hydrodynamic radius of 10 – 15 nm compared to 40-nm gold nanoparticles and 500-nm latex spheres) to permit unfettered study single-molecule properties within living cells. Despite these advantages compared to traditional optical markers and reporters, e.g., organic dyes, application of NQDs to the basic and applied biosciences remains limited by two factors: (1) Fluorescence intermittency (blinking) and (2) Sensitivity to the environment. These two intrinsic “flaws” derive from the same root cause – trapping of an excited-state carrier (electron or hole) at the NQD surface. In this study, we synthesized a NQD based on a graded inorganic shell approach to effectively confine the exciton (e-h pair) wavefunction to the nanocrystal core. All process was done in one pot by using the Successive Ionic Layer Adsorption and Reaction (SILAR) method.

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In-situ TEM Observation of Phase Transition in Confined Single-crystalline Ag_2Te Nanostructures

인준호, 유영동, *김현주, 김봉수

*KAIST 화학과 *KAIST 화학과*

We report the observation of thermal stress induced heterogeneous phase transition at the confined single crystalline Ag_2Te nanowires via in-situ electron microscopy. Unlike the phase transitions of bulk and freestanding nanowires, the confined nanowires showed the transformation into the body-centered-cubic structure along the interfaces to relieve the compressive stress by the suppressed thermal expansion. Furthermore, after the transition process, we observed the coexistence of high and low temperature phases at room temperature which seems to be ascribed by thermal stress. This work is the first result that exhibits the stress-dependent transition behaviors of Ag_2Te nanowires.

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새로운 형광체 Host인 $(Sr,Ca,Ba)_3(Al,Ga)O_4F$에 rare-earth activators가 치환된 형광체 연구

박상문, 최혜민, 장재성, 김혜진

신라대 에너지응용화학과

A new family of UV-activated phosphors made by substituting rare-earth activators such as trivalent Eu, Tb,Tm and Er into A_3MO_4F host lattices (A = Sr, Ca, Ba; M = Al, Ga) are introduced and their activation and emission spectra as well as their CIE values reported. The Tm-substituted system can be activated using light with a wavelength of 360nm. Relative intensities of a family of Tb-substituted green phosphors activated at 254 nm and with emissions centered near 548 nm are discussed.

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Synthesis of Y_2O_3:(Li,Eu) Films using Phosphor Powders Coated with SiO_2 Nano Particles

박철웅, *박상문, *박중철

*신라대 일반대학원 화학과 *신라대 에너지응용화학과*

$Y_{1.9-x}Li_{0.1}Eu_xO_3$ (x = 0.02, 0.05, 0.08, and 0.12) films were fabricated by spin-coating method. A colloidal silica suspension with $Y_{1.9-x}Li_{0.1}Eu_xO_3$ phosphor powder was exploited to obtain the highly stable and effective luminescent films onto the glass substrate. After heating as-prepared $Y_{1.9-x}Li_{0.1}Eu_xO_3$ films at 700 ^oC for 1 h, the phosphor films exhibit a high luminescent brightness as well as a strong adhesiveness on the glass substrate. The emission spectra of spin-coated and pulse laser deposited $Y_{1.82}Li_{0.1}Eu_{0.08}O_3$ films were compared. The cathodoluminescence of the phosphor films was carried out at the anode voltage 1 kV.

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Phosphorescent Organic Light-Emitting Devices with Branched Boron-Containing Ir(III) Electrophosphor: Lower Roll-Off Efficiency and Higher Doping Level

황동렬, 박수영

서울대 재료공학부

We report on a green electrophosphorescent Ir(III) complex with electron-transporting dimesitylboryl based branched substituents, iridium(III) bis[2-(2′-(dimesitylboryl)phenyl)pyridinato-*N*,$C^{2'}$]-acetylacetonato (Bppy2Iracac). Electrophosphorescent devices comprising this Bppy2Iracac:TPBi (TPBi = 2,2′,2″-(1,3,5-phenylene)tris(1-phenyl-1H-benzimidazole)) emitting layer exhibited external quantum efficiency as high as 5.25% at luminescence level of 10 000 cd/m^2, and significantly suppressed efficiency roll-off even in the driving current density beyond 100 mA/cm^2 due to the enhanced electron transporting property and balanced charge recombination. It was also found that the site isolation effect of emitting core by branched ligand allowed very high doping level of Bppy2Iracac up to 20 wt% into the host.

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Synthesis and Properties of Highly Fluorescent Room-Temperature Liquid Crystal Molecule

윤성준, 박수영

서울대 재료공학부

In the past decades, liquid crystals have attracted much attention in both industrial and academic fields due to their unique combined properties of molecular order and dynamics. In particular self-healing effect, which is combined liquid crystal (LC) property of molecular order and dynamics, reduces macroscopic domain boundaries and promotes the formation of a monodomain and enhances local arrangement of molecules. By this self-healing effect, LC materials exhibit the reorganization of the molecules into a more favorable packing, which is crucial for the device performance. Especially over the last decade, a great deal of attention has been paid on π-conjugated LC molecules because they have potential in applications as flexible optoelectronic materials. Several examples of π-conjugated LC molecules with photo- and electroactive functions have been reported, although practical application has been limited because of their high LC temperature region.Herein, we have synthesized a new cyanostilbene-based liquid crystalline material, (2Z,2'Z)-2,2'-(1,4-phenylene)bis(3-(3,4,5-tris(dodecyloxy)phenyl)acrylonitrile), GDCS, which forms LC phase at room temperature. GDCS shows very intense LC state fluorescence, due to the characteristic aggregation-induced enhanced emission (AIEE) process. In addition, we fabricated aligned LC microwires of GDCS by the micromolding in capillaries (MIMIC). We obtained an enhanced electrical conductivity of the LC aligned microwires, because the MIMIC process functions as a kind of rubbing effect on LC material.In this presentation, we will discuss the fundamental LC properties of GDCS, as well as the photo- and electroactive features.

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Synthesis and Properties of Highly Luminescent Infinite Coordination Polymer with Bistable Photoswitching

김진철, 윤성준, 박수영

서울대 재료공학부

In the past years, attention has been paid on photochromic materials related to their potential application in optical memory media. Among various photochromic compounds, 1,2-bis(thienyl)ethene (BTE) derivatives have been extensively investigated because of their high thermal stability, excellent photofatigue resistance, high sensitivity, and characteristic bistability. In particular, fluorescent photochromic materials, which are composed of photochromic unit and fluorophore combined by covalent bond, hold strong applicaton potential as ultrahigh density optical memory media. So far, we have reported a special class of fluorescent photochromic molecules, which show aggregation-induced enhanced emission (AIEE) as well as bistable photochromism in nanoparticles and polymer film.Herein, we have synthesized a new AIEE-active and photochromic infinite coordination polymer (ICP), which exhibits luminescence on/off switching reversibly and repeatedly. The mole ratio of photochromic unit and AIEE active unit in the ICP was varied to optimize the photochromic response. In addition, we effectively fabricated neat ICP film on the substrate by solution process. Erasable luminescence photoimaging on the neat ICP film was successfully demonstrated.

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Fluorescent Organic Nanowires :Synthesis, Self-assembly, and Device Fabrication

윤선우, 박수영

서울대 재료공학부

One-dimensional organic nanostructures such as nanowires, nanotubes and nanoribbons are attracting a lot of interest due to their great potential for construction of next-generation electronic devices. Fabrication of the nano-sized devices arrayed in molecular level is feasible by using self-assembly of the π-conjugated molecules. High mobility FETs devices are constructed when the molecules are well organized by π-π stacking.Herein, we demonstrate new π-conjugated molecules comprising dicyano-stilbene framework and aliphatic side chain. Attributed to their strong self-assemblying nature, uniform and fine nanowires could be easily formed by drop casting method. OTFT performance of these nanowires will be shown in this presentation .

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Design and Synthesis of Soluble 1,2,4-Linking Hyperbranched Poly(styrylthiophene) for Photovoltaic Applications

윤원식, 박수영

서울대 재료공학부

Polymer-based bulk-heterojunction solar cells are drawing considerable attention in recent years because of their easy fabrication, low cost, and the good possibility of obtaining flexible devices in comparison with traditional inorganic solar cells. [1] Most of the reported work on polymer photovoltaic cells has been investigated for the conventional π-conjugated linear polymer. However, the hyperbranched conjugated polymers have certain advantages over conventional linear conjugated polymers because of their unique structure. These polymers deserve attention in the field of photoelectronic devices, not only because of their good processibility but also because of their intramolecular energy/charge transfer properties.[2] In this work, we report on the synthesis and properties of a highly soluble and 1,2,4-linking hyperbranched poly(styrylthiophene) (1,2,4-hb-PT) prepared via Wittig reaction of A2 and B3 monomers. The 1,2,4-hb-PT were characterized using NMR, IR, GPC. The absorption spectra of 1,2,4-hb-PT showed distinct red-shifts compared to the conventional 1,3,5-linking hyperbranched poly(styrylthiophene) (1,3,5-hb-PT), attributed to the extended π-conjugation along ortho- (1,2-) and para- (1,4-) links. The inherent energy gradient from the shorter branches to the longer conjugated framework in 1,2,4-hb-PT enables characteristic energy funneling effect, which has been absent in conventional hyperbranched polymer of 1,3,5-hb-PT.[3] With this idea, we examined how the 1,2,4-hb-PT films behave in the solar cell application.

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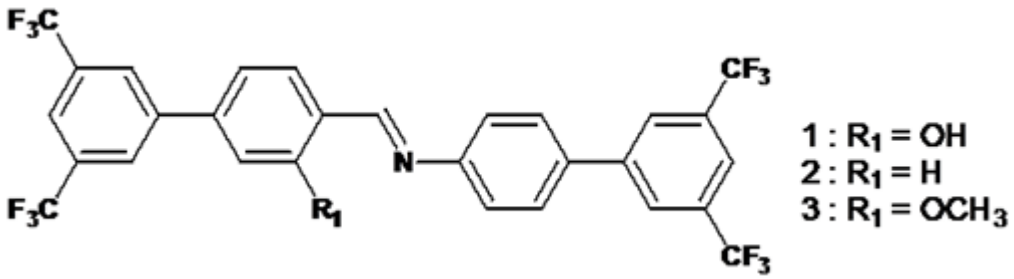
A Novel Salicylideneaniline-based Organogelator with Gelation Induced Emission Enhancement and Excited-State Intramolecular Proton Transfer

이종하, 권지언, 박수영

서울대 재료공학부

Recently, low molecular weight organic gelators(LMOGs) consisting of p-conjugated molecular framework are attracting considerable interest because of their multifunctional application potential. In this work, a novel class of highly fluorescent salicylideneaniline-based organic gelator (E)-4-((3',5'-bis(trifluoromethyl)biphenyl-4-ylimino)methyl)-3',5'-bis(trifluoromethyl)biphenyl-3-ol(AZTFBH, 1) has been synthesized. It has been found that 1 could gelate various solvents, such as dodecane, 1,1,2,2-tetrachloroethane, 1,2-dichloroethane and 1-octanol. Interestingly, the organogel showed enhanced emission compared to a solution of the same concentration and large Stoke's shift due to the occurrence of excited-state intramolecular proton transfer. Macroscopic and microscopic investigation by SEM and POM suggests that AZTFBH creates entangled three-dimensional networks consisting of the bundles of ribbon-shape fibrous aggregates. According to PL study, emission of gelated form is 25 times stronger than that of solution form. To investigate the role of OH part, 2 and 3 were additionally synthesized. It was found that OH group plays important role in the gelation process.



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Fabrication of Anodic TiO_2 nanotube arrays of controlled length for dye-sensitized solar cell (DSSC)

김상모, 이충혁, 김경하, 이완인

인하대 화학과

We fabricated TiO_2 nanotube array of various lengths and applied them to dye-sensitized solar cell (DSSC) as working electrode. For the synthesis of TiO_2 nanotube array, Titanium (Ti) foil was cleaned with a mixture of ethanol & acetone and then dried under nitrogen stream. Anodization was performed in a two-electrode configuration system with titanium foil as working electrode and platinum foil as counter electrode under constant potential at room temperature(25℃). A direct current power supply (DC 60V) was used as the voltage source to drive the anodization in an electrolyte contained ammonium fluoride (NH4F, 98+%; 0.5wt %) in Ethylene glycol (EG) in the presence of H_2O (2 vol %) for the period of 1-24hr with stirring speed of 150 rpm. In order to crystallize amorphous TiO_2 nanotube array into its anatase phase, two steps annealing process was carried out to remove organic solvents adsorbed on the surface of TiO_2 nanotube and to convert it into anatase phase. First, the calcinations at 150℃ for 2hr and then 450 °C for another 3 hr in the furnace. After all, a complete TiO_2 nanotube array of length 10 to 150μm & pore size of 100nm was obtained. We also studied the electron lifetimes (τe) and electron diffusion coefficients (De) of TiO_2 nanotube arrays for DSSC device using a stepwise phototransient with light source diode laser of 635nm. The overall efficiency of optimized TiO_2 nanotube array for DSSC device was obtained to be 6.0%.

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Solution phase chemical preparation of heterostructures of Ag and ZnO nanorods

박영석, 권태정, 채희권

서울대 화학교육과

Recently, the demands on modulating physical and chemical properties of nanostructures have drawn the emerging interest in the hybrids between plasmonic nanoparticles and semiconducting nanostructures. Ag-ZnO heterostructures have been of particular interest due to the highly efficient photocatayltic activity, which were elucidated to arise from the energy transfer between metallic nanoparticles and ZnO nanostructures, and metallic nanoparticles on the surface of ZnO were found to be capable of manipulating the optical properties of ZnO nanostructures. But the relationship between the resulting hybrid structures and the improved photocatalytic performance were still not fully understood. Thus, it remains challengeable to develop the novel heterostructures of two distinguishable materials and to observed their properties. Herein, we described the solution phase synthetic strategy to make use of carboxylates as surface modifiers, and consequently the multiple growth of Ag nanoparticles on the surface of ZnO nanorods was induced by chemical reduction in solution phase.

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A Graphene-based Platform for DNA Unwinding Activity Assay of SARs CoV Helicase

장홍제, 김영관, *여운석, *김동은, 민달희

*KAIST 화학과 *건국대 생명공학과*

Helicases are a class of essential enzymes that unwind double stranded into single stranded nucleic acid. The unwinding of DNA is a key reaction for all single stranded DNA required processes such as cell proliferation and viral replication. Due to their critical role in viral process, helicases have been targeted for therapy in many virus diseases. Therefore, it is important to develop a simple, fast and cost-effective platform for helicase unwinding activity assay. Herein, We developed graphene oxide (GO) based platform for helicase activity assay. The strategy relies on preferential binding of GO to single stranded DNA over double stranded DNA, thereby quenching fluorescence of dye labeled single stranded DNA. Our GO based strategy enabled real-time monitoring and quantitative assay of DNA unwinding activity. In addition, the GO based platform is compatible with high-throughput screening of helicase inhibitors. We expect that our GO based helicase assay method will be one of the most convenient and efficient helicase assay systems with cost-effectiveness and simplicity.

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The Growth of Gold Rods on Supported Graphene Films for the Development of Novel Graphene Based Nanohybrid Structure

김영관, 장홍제, 한상우, 민달희

KAIST 화학과

Graphene, a single layered sp2 carbon network compacted into a two-dimensional honeycomb lattice, has extensively attracted much attention due to its fascinating electronic, mechanical and optical properties. Therefore, many efforts were devoted to prepare nanohybrid structures of graphene with noble metal nanoparticles to improve their own functionalities for various applications. Nanohybrid structure of graphene with one dimensional gold nanostructure, such as rod and wire, has been less explored than that with particle in spite of its potentially useful properties including dimensional dependent optical properties of gold nanostructures. In this work, we describe a simple direct growth method of one dimensional gold nanostructure on supported graphene thin films via both seed-mediated and seedless approaches. The fabricated nanohybrid thin film showed significant Raman signal enhancement of graphene by 34-folds at the tip of gold nanorod. To the best of our knowledge, this work is the first example of engineering nanohybrid structure of graphene and one dimensional gold nanostructure through direct growth of gold structures on graphene surface. We believe this nanohybrid thin film will be a promising candidate for novel surface enhanced Raman platforms and nanoelectronic devices.

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Polyelectrolyte Multilayer Growth Revisited by Introducing a Rugged Multilayer Template as Substrate

MD. ARIFUR RAHIM, *이하진, **전일철

*전북대 나노기술학과 *한국기초과학지원연구원 전주센터 **전북대 화학과*

Pristine polyelectrolyte multilayer (PEMs) composed of poly(allylamine hydrochloride) (PAH) and poly(sodium 4-styrenesulfonate) (PSS) were treated with anionic surfactant to obtain rough and porous templates by the surfactant induced PE desorption from the pristine film. These templates served as the base substrate for fresh multilayer buildup of the same polyelectrolyte pair. Salt free and salt (NaCl) containing growth solutions were used for the fresh multilayer formation. The growth behavior was found to be much different from the conventional growth on relatively flat surface and dependent on the effective electric field induced by the template at the interface as well as the surface cavities with their intrinsic charge distribution. Moreover, both the films showed nonlinear and linear growth regimes but maintained different surface morphologies compared to the template or the pristine film. UV-Vis absorbance spectroscopy, zeta potential measurement, atomic force microscopy (AFM) and transmission electron microscopy (TEM) were employed to study the entire system. These findings might add a different flavor to the usual model of the PEM growth and can lead to an alternative route for PEM construction with different architecture.

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Application of quantum-dot sensitized solar cells with sub-micron-sized TiO_2 spheres

성상도, 한송이, 엄재호, 이완인

인하대 화학과

The effect of TiO_2 structure on the performance of quantum-dot sensitized solar cell (QDSSC) has been investigated with sub-micron sized nanoporous TiO_2 sphere and P25. Monodispersed 350 nm-sized TiO_2 sphere with ultra-high surface area and hierarchical pore structures was synthesized by sol-gel reaction and a specially-designed hydrothermal treatment with titanium isopropoxide in a co-solvent condition with amine as a basic catalyst. The prepared nanoporous TiO_2 sphere and P25 were applied as a photoelectrode in the QDSSCs. The fabricated QD-sensitized photoelectrodes from them have been prepared by sequential deposition of Cadmium sulfide (CdS), cadmium selenide (CdSe) and zinc sulfide (ZnS) quantum dots on the TiO_2 electrodes by a chemical bath deposition (CBD) method. The photovoltaic performance achieved from nanoporous TiO_2 was ~ 30 % higher than that of QDSSC from the P25 due to their high surface area and efficient hierarchical pore structure.

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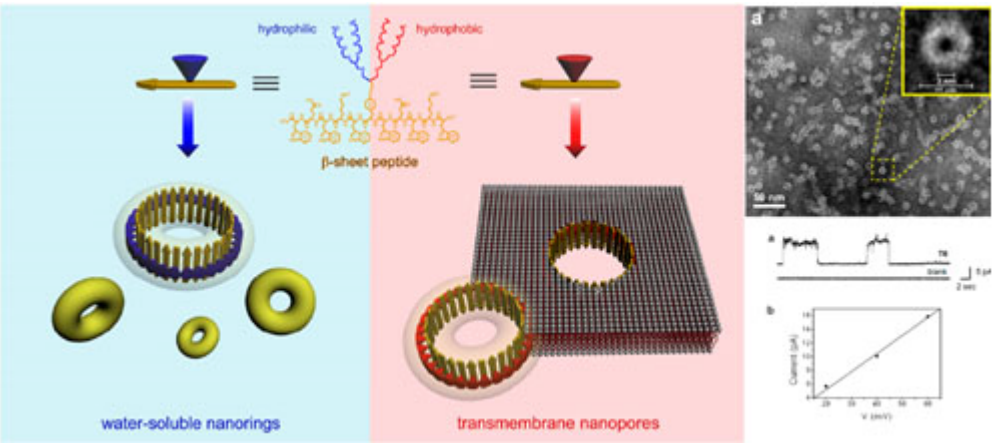
Formation of barrel-like structure from self-assemblinhg dendrimeric β-sheet peptides

박일수, 이명수

서울대 화학과

An interest in artificial bionanosturctures has been intense and is expected to escalate further. Recently, we have described a rational approach to construct artificial β-barrel proteins from the self-assembly of peptide-based building blocks. With this approach, the direction of self-assembly process to the formation of water-soluble β-barrel nanorings or water-insoluble transmembrane β-barrel pores could be controlled by the simple but versatile molecular manipulation of supramolecular building blocks. We have explored that T-shaped β-sheet peptides with hydrophilic dendrimer formed nanorings in KF solution. On the other hand, same shaped peptides with hydrophobic dendrimer make pores in lipid bilayer, even though it cannot self-assemble into any structure in water. By proton transport experiment, we have confirmed that these peptides could construct holes between membranes. Therefore, we can manipulate a specific structure such as barrel-like structure by controlling β-sheet conformation as a rod and curvature by dendrimer.



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Polyelectrolyte Multilayers-Based Tunable Nanoreactor for Synthesizing Nanomaterials with Controllable Properties

고혜아, *이하진, *배태성, *최원산

*충남대 분석과학기술대학원 *한국기초과학지원연구원 전주센터*

Since their discovery on 1997, polyelectrolyte multilayers (PEMs) have been considered as a potential tool for preparing nanocomposites or nanostructures. Polyelectrolyte multilayers (PEMs) can be fabricated onto charged melamine formaldehyde (MF) colloidal particles by stepwise adsorption of oppositely charged polyelectrolytes via layer-by-layer (LbL) self-assembly technique, referred to as a PEM-coated particles (PEMPs). Inorganics synthesis (SiO_2 or iron oxide) within PEMPs can be carried out by loading precursors into PEMs, followed by a chemical treatment. Heat treatment of the resulting particles leads to formation of hollow structures consisting of SiO_2 or iron oxide only. After incorporation of ionic polymers into the capsules, such capsules could be utilized as special nanoreactor for synthesizing tailored nanomaterials with controllable properties. Size of hollow structures can be also tuned by varying the template sizes, which means that it is able to control the reactions in confined environment. If this can be achieved, it might open up a new route to the development of tunable nanoreactor, which could control a variety of chemical reaction.

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Controlling polymorph and Crystal Shape of TiO_2 Nanoparticles by Simple Hydrothermal Method

권도훈, 김영일

부경대 화학과

Nanosized TiO_2 of both anatase and rutile phases were synthesized by acidic hydrolysis of titanium isopropoxide and subsequent hydrothermal treatment. It has been earlier known that the type of acid uesd in the synthesis had a major impact on which polymorph of TiO_2 structure: HCl gave rutile structure of the titania, whereas HNO_3 did anatase. In this study we will show that controlling only pretreatment method and hydrothermal reaction time can change the structure of TiO_2 from anatase to rutile in HNO_3 media. The crystal shapes of the synthesized TiO_2 can be also changed from nanoparticle to nanorod.

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Synthesis of Plate like silver particles

이채성, *김호건

*한양대 응용화학과 *한양대 화학과*

본 연구에서는 금속염(silver nitrate)을 출발 물질로 하여 중간 생성물(silver cyanate)을 이용한 화학적 환원법으로 은 입자를 제조 하였다. 금속염(silver nitrate)와 urea 의 반응에서 중간 생성물인 silver cyanate 가 판상의 형태로 형성되었고, silver cyanate 의 형상을 반영한 은 입자를 얻기 위해 강력한 환원제인 sodium borohydride 를 사용하였다. 그 결과 ethanol 용매에서 80℃/60 분 이상 반응 하였을 때 판상의 silver cyanate 를 얻을 수 있었고, 환원제(sodium borohydride)의 농도가 3x10^-3mol 일 때, 40um 크기를 갖는 판상의 순수한 은 입자를 얻을 수 있었다.

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The Stacking Structure of Poly (Styrene-co-Butadiene) Composites with the Graphite Oxide for the Gas Barrier Properties

윤상천

KAIST 생명화학공학과

We report here a novel method for the fabrication of composites which have a stacking structure with the SB copolymer and polystyrene-graphite oxide (PS-GO). This process uses two steps for fabrication of the composite films. The first step is that the GO is dispersed in the SB copolymer matrix. We are attached to the PS on the GO surface for good dispersion in the solution of SB copolymer. The second step is the fabrication of composite films of SB copolymer with PS-GO. The SB copolymer has a lamellar structure because they have 45 wt % polystyrene (PS) by self-assembly. The PS-GO is embedded in the styrene parts in the SB copolymer. The suspension of SB copolymer and PS-GO is poured in the Teflon dishes, and then the solvent is evaporated at the room temperature, finally we obtain the films of the SB copolymer composite with PS-GO. This strategy leads to the formation of a stacking structure for the gas barrier properties. The graphite oxide is enhanced to the gas barrier properties due to a plate structure and absorption properties of graphite oxide. These composites have a long pathway and absorption properties, so they are less gas permeability than pure SB copolymer. This method is cost-effective and it can be large mass production. We suggest that it is possible to enhance the gas barrier properties with GO.

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Preparation of mesoporous silica as nanogate immobilized Benzo-18-Crown-6

최영란, 박경원, 정종화

경상대 화학과

Benzo 18-crown-6 was immobilized onto the surface of SBA-15 by sol-gel grafting reaction in toluene. Benzo 18-crown-6 immobilized SBA-15(B18C6-SBA-15) was characterized by SEM, TEM, FT-IR and solid ^{13}C-NMR. 20 wt % of Benzo 18-crown-6 was attached by measurement of TGA. B18C6-SBA-15 formed complex with alkyl diammonium ion by the hydrogen-bonds. In this conference, we will explain on preparation of B18C6-SBA-15 in detail.

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IrO_2-$Ru(DABP)_3^{2+}$ System for Photochemical Water Oxadation

윤용태

부경대 화학과

IrO_2 - $Ru(bpy)_3^{2+}$ system has been studied for photochemical water oxidation. IrO_2 colloid as water oxidation catalyst was synthesized and characterized by TEM, XRD, XPS and UV/Vis spectroscopy. The synthetic time and temperature affected the characteristics of IrO_2 except the size of the particles. To control the redox potential and light absorption, the ligand of $Ru(bpy)_3^{2+}$ should be modified by derivitization. It was expected that appropriate derivatization can make more effective electron transfer between colloidal IrO_2 and bipydiryl ruthenium complex. $Ru(DABP)_3^{2+}$(DABP : 4, 4'-diamino-2, 2'bipyridine) was synthesized and its characteristics for photochemical water oxidation was compared with $Ru(bpy)_3^{2+}$.

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Synthesis of SrY_2S_4:Eu Phosphors in a Closed System by Using Quartz Ampule with Flux-Aided Solid-State Reaction.

오지혜, 도영락

국민대 생명나노화학과

We synthesize the SrY_2S_4:Eu phosphor powders using SrS, Y_2S_3, EuS, S, and flux to decrease reaction time. The starting materials were mixed in a mortar in Ar atmosphere and calcinated in a quartz ample, which was sealed under 10^{-3} torr vacuum atmosphere. We can decrease the reaction time and temperature, prevent oxidation of starting materials, and synthesis without gas flow such as H_2S during the reaction time by using the quartz ampule. The optical properties of SrY_2S_4:Eu shows a red emission, which is located at ~630nm with excitation at 365nm, and the crystalline properties shows orthorhombic phase for $CaFe_2O_4$ structure. The crystallographic structures, optical properties, and morphology of the SrY_2S_4:Eu with various kind of fluxes were characterized by X-ray diffraction (XRD), Photoluminescence (PL), and Scanning Electron Microscopy (SEM) measurements.

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Optical properties of sol-gel derived $Y_2O_3:Er^{3+}Yb^{3+}$ upconversion Red thin-film phosphor on sapphire substrate

박병규, *도영락

*국민대 화학과 *국민대 생명나노화학과*

Red upconversion luminescence of flux($LiCO_3$) contained Er^{3+} and Yb^{3+} codoped Y_2O_3 thin-film phosphors have grown on a sapphire substrate using a Pechini-type sol-gel process by employing Yttrium nitrate, Erbium nitrate, Ytterbium nitrate, Citric acid as precursor materials. $Y_2O_3:Er^{3+}Yb^{3+}$ exhibit strong Red upconversion luminescence under the excitation of a 978nm IR laser. To enhance optical properties of $Y_2O_3:Er^{3+}Yb^{3+}$ thin-film phosphors, we studied various preparation condition, such as annealing temperature and flux concentration. Structural and optical properties were investigated by X-ray Diffraction (XRD), Atomic Force Microscopy(AFM), Scanning Electron Microscopy(SEM) and Photo luminescence(PL)

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Field Emission of High-Quality ZnO-Nanorods By Hydrothermal-Electrochemical Deposition(HED)

박재형, *도영락

*국민대 화학과 *국민대 생명나노화학과*

The well-ordered ZnO nanorods can be used as electron field emission arrays. High-quality ZnO nanorods with low defect concentrations were grown on ZnO seed-layer-coated Pt/Si substrates by means of electrochemical synthesis under relatively high temperatures (

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Wetting properties of artificially fabricated various superhydrophobic surfaces

박후근, 도영락

국민대 생명나노화학과

Superhydophobic surfaces can be achieved with a water contact angle higher than 150° by generating rough surfaces coated with low surface energy molecules. Various rough surfaces were fabricated on quartz substrates with several kinds of rod geometries by changing the diameters, space to diameter ratios and heights. Various nanospheres were used for fabricating such rough surfaces through nanosphere lithography. Teflon used for low surface energy coated on various rough surfaces by spin-coating. wettability of their surfaces could be modulated from superhydrophilic to superhydrophobic by modifying them with coating of teflon. The structural, morphological and wetting properties of superhydrophobic surfaces were investigated by performing scanning electron microscopy (SEM), atomic force microscopy (AFM) and contact angle measurements.

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Enhancement forward efficiency of $Y_3Al_5O_{12}$:Ce phosphor-based white light-emitting diodes using light recycling filter

오정록, *도영락

*국민대 화학과 *국민대 생명나노화학과*

We have investigated a simple approach for the design of blue excitation light passing and phosphor-yellow-emission-light reflecting dielectric multilayers to recycle the backward emission of $Y_3Al_5O_{12}:Ce^{3+}$ (YAG:Ce) yellow phosphors on top of a blue InGaN light-emitting diode (LED) cup. The Light Recycling Filter(LRF) consisting of alternating layers of TiO_2 and SiO_2 is added between a YAG:Ce phosphor layer and glass substrate. Results show that the light extraction efficiency and luminous efficacy is higher than that of conventional LEDs by 164% and 195%, respectively, and the correlated color temperature becomes lower, below 4000 K

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Photoelectrochemical water decomposition for coupled semiconductor by 4-mercaptobenzoic acid modified TiO_2 nanotubes with CdS

박수정, *이성훈

*서울대 나노융합학과 *서울대 화학부*

The highly ordered hole-array materials formed by electrochemical anodization of various valve metals have been a great deal of interest due to unique geometrical structures, facile fabrication process, economic feasibility, and a wide range of applications in the field of nanoscience. Among them, titanium oxide (TiO_2) nanotube arrays are used as a photoanode in the photolysis of water, due to the excellent properties such as high aspect ratio, the proper band gap position, and photo-stability. However, the limitation in the application of the highly ordered TiO_2 nanotube arrays as a photoanode in the split of water is the large band gap. That is, the highly ordered TiO_2 is only photoresponsive to a UV region. To expand photocatalytic activity to visible light, mercaptobenzoic acid derivatives to tether CdS to TiO_2 is necessary.We reasoned that the phenylene groups of these linkers would provide increased electronic coupling and more precisely defined interlayer separation.Here, we reported on investigated the relationship between water splitting behavior and the CdS through chemical bath deposition method to 4-mercaptobenzoic acid modified highly order TiO_2 nanotube arrays exhibited enhanced photocurrents under a simulated AM1.5 illumination.

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Controlled overgrowth on Au nanorods through site-specific functionalization

송재희

순천대 화학과

Au nanorods were used as seeds for the controlled overgrowth of thin shell of gold or silver by using a mild reducing agent, ascorbic acid in the presence of cetyltrimethylammonium bromide at ambient conditions. We could tailor the growth of sheathes of gold and silver on gold nanorods via site-specific functionalization on Au nanorods. Before we grew thin sheath of Au or Ag, the surface of gold nanorod seeds was modified so that the sheath crystal could grow favorably to the direction of {110} planes of the seeds.

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A new synthetic approach for the synthesis of Au-Ag composite nanorods

송재희, 고인혜

순천대 화학과

A synthetic procedure is presented for the production of Au nanomaterials via a simple proton beam irradiation process. It was found that the size and shape of the prepared gold nanomaterials using proton beam irradiation were easily controlled by the concentration of silver ions, which was added to the Au growth solution. As the concentration of silver ions was increased, there was an apparent increase in the aspect ratio of Au nanorods. From EDS analysis, the nanorods were found to be composed of ~90 % gold and ~10 % silver.

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Photovoltaic properties of conjugated organic dyes containing alkylthio-substituted thiophene for DSSCs

사공천, 문주석, 김재필

서울대 재료공학부

We reported the design and synthesis of a series of conjugated organic dyes that contain N,N-bis(4-hexyloxyphenyl)aniline as donor and cyanoacrylic acid as acceptor (anchoring group). These two moieties were bridged by alkylthio-substituted thiophenes, such as 3,4-Ethylenedithiothiophene (EDTT), 3-(3-methyl-butylthio)thiophene (3MBTT) or 3,4-bis(3-methyl-butylthio)thiophene (B3MBTT). Their photovoltaic performance was estimated under standard global AM 1.5 solar condition.

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Electrochemistry and Fluorescence of Pyrene Labeled Gold Clusters

곽규주, *Mary Sajini Devadas, 박정우, 최지환, 전철호, *Ramakrishna Guda, **이동일

*Department of Chemistry, Yonsei University *Department of Chemistry, Western Michigan University*
***Department of Chemistry, Yonsei University Department of Chemistry, Western Michigan University*

We present synthesis and electrochemical and optical properties of chromophore-functionalized gold clusters, which have practical implications in solar energy conversion, sensors, and optical applications. Pyrene labeled gold clusters were synthesized by exchange of the thiolated pyrene (PySH; N-(2-mercaptoethyl)pyrene-1-carboxamide) onto hexanethiolate capped gold clusters and characterized using transmission electron microscopy (TEM), electrochemical voltammetry, UV-vis absorption and fluorescence spectroscopy. It is found that the fluorescence of pyrene is dramatically quenched upon binding to gold clusters. This results suggest that pyrene and gold clusters have strong excited-state interactions. The origin of these effects is considered to be the electron transfer from gold clusters to attached pyrene. The square wave voltammetry of pyrene labeled gold clusters shows that the first oxidation potential of gold clusters is shifted to more positive value. This means that gold clusters become more difficult to be oxidized when pyrene is attached, indicating directional electron flow from gold clusters to pyrene. These results are compared with well-defined ferrocene-pyrene dyad systems.

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ZnO/ZnSe/CdSe Core-Shell Nanocable Arrays Synthesized by Chemical Vapor Transport

명윤, 박정희

고려대 소재화학과

High-density ZnO/ZnSe/CdSe core-shell nanocable arrays were synthesized on large-area Ti substrates. The outer layers were deposited on the pre-grown vertically-aligned ZnO nanowire arrays, with a controlled thickness (10~50 nm), using the chemical vapor transport method. Their shell composition controlled by growth temperature and reaction time. The structural and optical analysis suggests the formation of CdZnSe alloy in the interface region between the ZnO core and CdSe shell, which would enhance the charge separation by reducing the lattice mismatch. Therefore, the photoelectrochemical cell using the ZnO/ZnSe/CdSe photoelectrode exhibits much higher photocurrent and hydrogen generation rate than that using the ZnO-ZnSe one.

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Laminated Composite of Thermoelectric Oxide prepared by Exfoliation and Heterogeneous Nucleation

정희성, 김종영

한국세라믹기술원 이천분원

Laminated composite of cobalt oxide and heterogeneous oxide such as calcium oxide was fabricated by exfoliation of NaxCoO2 and subsequent heterogeneous nucleation, which results in increased Seebeck effect by quatum well effect.

대한화학회 THE KOREAN CHEMICAL SOCIETY

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The Effect of Surface Modification on Electrochemically Deposited Metal Chalcogenide Film

정희재, 김종영

한국세라믹기술원 이천분원

Multilayered thin film of metal chalcogenides, copper-indium-selenide(CIS) and cadmium sulfide(CdS), was fabricated by electrochemical and wet solution process. The deposition process and microstructure were investigated in relation to surface modification of substrate via plasma treatment.

THE KOREAN CHEMICAL SOCIETY

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Titanium oxide Nanoparticles - decorated Zinc Oxide Nanowires for P-type Devices.

김창현, *김준동, 명윤, 성태광, **한창수, 박정희

*고려대 소재화학과 *한국기계연구원 나노융합기계연구본부 **한국기계연구원 나노공정장비센터*

The heterostructures of titanium oxide Nanoparticles (TiO)-decorated zinc oxide (ZnO) nanowires were synthesized and applied for ultraviolet (UV) sensors. ZnO nanowires were grown on a nickel (Ni) foil by a chemical vapor deposition method. Various thick Ti films were coated around the grown ZnO nanowires. Rapid thermal treatment was performed, which causes phase changes of TiOX(x

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Synthesis of CIGS absorber layers via a ink coating by solvothermal route.

조진우, *김웅

*고려대 신소재공학과 *고려대 신소재공학부*

Non-vacuum processes have been suggested to solve the problems of the current CIGS solar cell fabrication methods, such as printing, electroplating, spraying, etc. $Cu(In_xGa_{1-x})Se_2$ (CIGS) nanocrystals were prepared by a ink coating with the aim of developing a simpler and the lower cost method for fabrication the absorber layers of thin film solar cells. Recent progress in the solvothermal synthesis of high quality nanocrystals have new routes for the fabrication of low-cost efficient photovoltaic devices. Chalcopyrite copper indium sulfide ($CuInS_2$) and copper indium gallium selenide ($CuIn_xGa_{1-x})Se_2$) nanocrystals were synthesized by arrested precipitation in solution. The In/Ga molar ratio in the CIGS nanocrystals could be controlled by varing the In/Ga reactant ratio in the reaction. The compositional and structural characteristics of nanocrystals and films were investigated by various analysis techniques including SEM, TEM, XRD, and EPMA, and will be discussed in the presentation.

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Fabrication of DSSCs using TiO2 inverse opal photoelectrode For Enhanced Light harvesting Efficiency

서영곤, *이현정, 이원목

*세종대 화학과 *KIST 고분자하이브리드센타*

본 연구에서는 광결정 TiO2 광전극 기판을 제작하여 입사광을 가두는 광증폭 효과로 염료의 빛 흡수율을 높여 염료감응형 태양전지의 효율을 증가시키는 연구를 수행하였다. 광결정 TiO2 전극은 비교적 짧은 시간에 대면적 TiO2 inverse opal film 을 만들 수 있는 slide coating 방법으로 제작하였다. Sol-gel 합성과 peptization 반응을 통해 약 8nm 크기의 잘 분산된 TiO2 입자들을 얻었다. 그 TiO2 나노입자 분산액은 수열 처리과정을 거쳐 약 20-30nm 의 크기로 늘어났지만 결정성과 굴절률이 상당히 증가하였으며 분산도와 thin film 에서의 투명도는 유지되었다. 이렇게 합성된 TiO2 나노입자는 여러 가지의 유화중합 조건으로 합성된 다양한 크기의 PS 희생입자와 혼합되고 slide coating 의 방법에 의해 FTO 기판에 coating 되었다. 이어지는 calcination 과정을 통해 TiO2 inverse opal electrode 가 제작되었다. TiO2 inverse opal film 들을 염료감응형 태양전지 광전극으로 활용하여 효율 향상을 관찰하였다. 또한 다양한 크기의 PS 희생입자를 사용하여 TiO2 inverse opal films 의 pore 크기를 조절할 수 있었으며 그에 따라 광증폭을 위한 빛의 파장도 조절하였다.

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Synthesis of One-Monomer-Thick Two-Dimensional Polymers

황일하, 백강균, 이다미, 윤경원, Raghunandan Hota, 김기문

포항공과대 지능초분자연구단, WCU 첨단재료과학부, 화학과

Synthetic two dimensional (2D) polymers are expected to have on many fundamental and applied aspects of the natural and engineering sciences. Although numerous approaches have been reported over the last several decades, the synthesis of a one-monomer-thick, covalently bonded 2D polymer with a long-range ordered internal structure has yet to be achieved. Here we present a novel synthetic method of 2D polymers on gold surface via the cross metathesis of $(allyloxy)_{12}$cucurbit[6]uril or Zn-(4-pentenylthio)$_8$phthalocyanine. The resulting polymers were characterized by various techniques including IR, UV/Vis, and TEM. In addition, characterization of the 2D polymers after transfer onto Si wafer with PDMS stamp will be presented.

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리튬흡착제 스피넬형 망간산화물의 첨가원소 및 첨가량에 따른 영향

김양수, *류현주, *송혜정, *양경모, *김정준, *이우람

*한국기초과학지원연구원 순천센터 *전남대 화학과*

해수로부터 나노 크기의 Li 원소를 흡착하는 여과·분리기술은 발전에 발전이 계속 되어 오고 있다. Li 나노물질을 여과하기 위한 물질 중의 하나인 망간산화물은 나노이온 분자의 여과뿐만 아니라 촉매로의 가능성이 높다고 알려져 있다. 본 연구에서는 좋은 양이온 교환능력을 보이는 나노물질여과 흡착제의 합성을 기존의 수열방법과는 달리 고상반응법을 통해 첨가원소 및 첨가원소의 함유율에 따라 제조하였다. 이 반응은 기존의 액상반응법이 아닌, 대량생산이 용이한 고체상태의 시료로써 반응시키기 때문에 주목할 만한 의미가 있다. 본 연구에서는 기존에 Li1.6Mn1.6O4 에 Fe, Ni, Co, Cu, Ti 원소들을 첨가하여 각 원소 및 원의 함유율(%)에 따른 Li1.6[Mn% X%]1.6O4 화합물을 제조하여 비교 분석하여 이를 통한 최적의 흡착능을 얻을 수 있는 흡착제 제조조건을 확립하고자 한다.

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CN_x (x=0-10%) Layer Deposition on Vertically-Aligned Silicon Nanowire Array: Enhanced Conductivity Applied for Feield Emission Display and lithium-ion battery anodes

조용재, 정경복, 김창현, 김한성, 명윤, 박정희, *조재필

*고려대 소재화학과 *울산과학기술대 에너지공학부*

Vertically-aligned silicon nanowire (Si NW) arrays at a large area of silicon substrates, with desirable axial crystallographic orientation were synthesized by a facile metal-nanoparticle-assisted catalytic etching technique. Carbon and N-doped carbon (CN_x, x=0-10%) layers deposited on the Si NWs via the subsequent carbon deposition using a pyrolysis of methane, with a controlled thickness in the range of 10-50 nm. The N content was increased up to 10 at. %, with a dominant pyridine-like structure. The current mode measurent in the atomic force microscopy and Terahertz spectroscopy were employed to elucidate the enhanced electrical conductivity of 50 nm thick outerlayers at least by a factor of 2, for the deposition of CN_x outerlayers. The field emission and lithium ion battery shows the largly enhanced conductivity effect of the thicker outerlayers, but negligibly depending on the N incoporation. The field emission desplays shows 1.4 mA/cm^2 at 8 V/μm, and the lithium ion battery shows the storage ability as high as 1060 mAh /g after 45 cycles.

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Inverse Opal Structure Film: Method of Manufacturing as Scattering Layer in Dye-sensitized Solar Cells

김명실, 김성수, 김지만

성균관대 화학과

Dye-sensitized solar cells, one of the most attractive energy sources to alternate fossil fuel, are improved its light conversion efficiency by various method for several years. Among these improvements, concentration of light by a scattering layer is much effective. The inverse opal TiO_2 electrodes which are synthesized by self-assembled using sphere materials such as PMMA, Polystyrene and Silica Spheres lead to higher light harvesting efficiency. The inverse opal TiO_2 electrodes have been considered due to their photonic crystal characteristics and light scattering effect. It caused a significant change in dye absorbance which depended on the position of the stop band 200nm to 600nm. However, these inverse opal TiO_2 electrodes have a crucial problem for DSSCs system because of insufficient adsorption amount of dye due to their low surface area. In this study, we synthesized mesoporous inverse opal TiO_2 electrodes to increase their surface area for abundant dye adsorption. The photo-conversion efficiency of the DSSCs with mesoporous inverse opal TiO_2 electrode as a light scattering layer has increased compared to that of inverse opal TiO_2 electrode DSSCs.

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Dual Functionality of Mesoporous TiO2 Film as Light Scattering Layer in Dye-sensitized Solar Cell

김성수, 김명실, *이윤연, 김지만

*성균관대 화학과 *성균관대 나노과학기술협동학부*

Dye-sensitized solar cell (DSSC) is regarded as a regenerative low-cost alternative to conventional devices. To increase photo-current density, bi- or tri-layer structure film using various size and type TiO2 particles is fabricated as a light scattering layer such as sphere, hollow and inverse opal. However, these materials is too restriction of dye adsorption for enhance photo-conversion efficiency. A dual functional material with performed enough adsorption amounts of dye and light scattering role is required to overcome limitation of pre-existence materials and go for high performance DSSC. Here, we modify the application of mesoporous TiO2 particles which is synthesized by nanocasting method from mesoporous silica template as a light scattering layer in dye-sensitized solar cells. The light scattering layer using mesoporous TiO2 particles shows that it has much adsorption amount of dye by high surface area which is the representative characteristic of mesoporous material and also light scattering effect by its particle size around 200 nm spheres. This dual functionality of mesoporous TiO2 particles suggests new advance for high photo-conversion DSSC.

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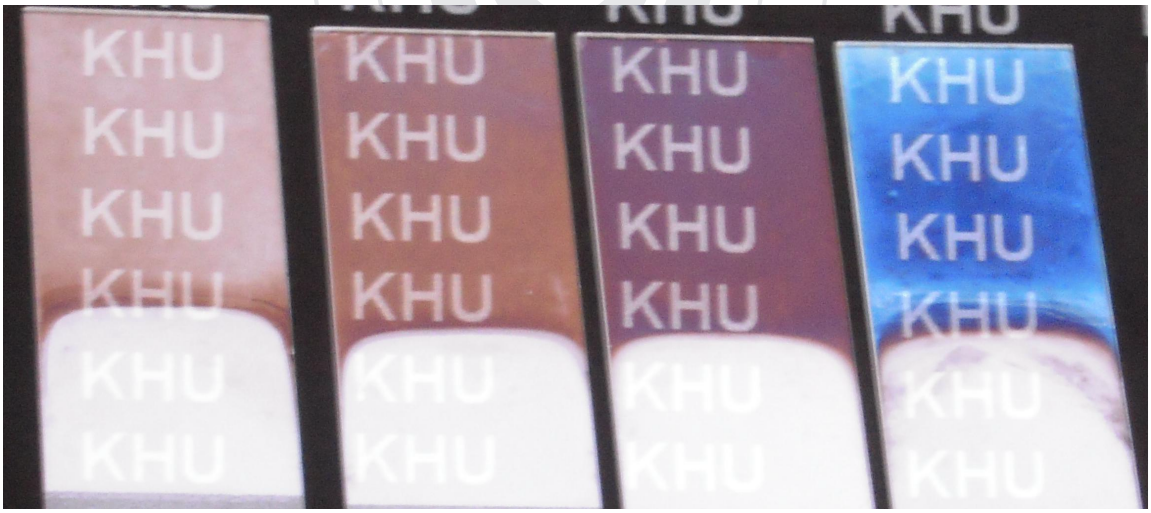
Anti-Reflective coating of La(OH)3 rods

유지호, 원화영, 변송호

경희대 화학과

La(OH)3 suspension produced from hydrolysis of LaOCl. And coating glass by using La(OH)3 suspension. Coating method is dipping process. Coated glass has "Anti-Reflective property".Transmittance graph shows "Anti-Reflectivity",and coated glasses more translated light than uncoated glass.



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Silica Nanoparticle Assisted Synthesis of Mesoporous Crystalline Metal Oxides with Controllable Pore Size

이윤연, *이형익, **이기림, **권영욱, **김지만

*성균관대 나노과학기술협동학부 *University of California, Santa Barbara, USA **성균관대 화학과*

Herein, we developed totally novel approach, based on the interaction between silica nanoparticles with metal oxide nanoparticles which produces mesoporous metal oxides with crystalline walls and controllable morphological features including the porosity. At an appropriate solution pH, the smaller silica nanoparticles are attached to the surface of the larger metal oxide nanoparticles and dictate the direction and the degree of condensation of the metal oxide nanoparticles, resulting in a porous 3D framework. Crystallization by a hydrothermal treatment and removal of silica nanoparitcles with sodium hydroxide solution result in a meosporous metal oxided with crystalline walls. The porosity can be controlled in the ranges of 8-35 nm of mean pore diameter in case of titania by the relative amounts of the nanoparitcles.

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The selective bind of thiolated Multi-Walled carbon nanotubes and Gold-Nanoparticles through covalently bond.

이병욱, 김영준, *송재희

*충남대 화학과 *순천대 화학과*

Multi-Walled Carbon Nanotubes(MWCNTs) surface was modified through the oxidation using strong acid such as HNO_3 and functional groups were introduced. In this study, thiolated MWCNTs were preparated via the reaction of oxidized MWCNTs and aminothiol. Gold nanoparticles(AuNPs) were selectively attached to the thiolated nanotubes. We compared the shape of pristine MWCNTs-AuNPs with thiolated MWCNTs-AuNPs. The binding energy of sulfur atoms in thiolated MWCNTs and AuNPs was compared using X-ray photoelectron spectroscopy. The characterization of nanocomposites has been done by using TEM, FT-IR, and so on.

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Terahertz Absorption and Emission from Vertically-Aligned Silicon Nanowire and Silicon-Carbon Core-Shell Nanocable Array

서영석, 정경복, 조용재, 명윤, 김한성, 박정희

고려대 소재화학과

We synthesized vertically-aligned p-type and n-type silicon nanowire arrays on a large area of silicon substrates, with a desired diameter, length, and crystallographic orientation, using by a metal-nanoparticle-assisted catalytic etching technique. The length was controlled from 500 nm and 3 μm. We observed the terahertz (THz) emission from these Si nanowires (NWs) excited by a 100 fs pulse of 810 nm radiation from a Ti:Sapphire laser system, and compared it with that of a Si film. The frequency spectrum (0-4 THz) of the THz emission from the Si NWs is red shifted by 0.2 THz. This red shift is though to originate from the anisotropic nanowire geometry, which causes a decrease of the longitudinal plasmon oscillation frequency. The graphite layers were subsequently deposited on the silicon nanowire array using a pyrolysis of acetylene. We observed that the graphite deposition enhances significantly the THz absorption, owing to their increased conductivity.

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Effect of Framework Polarities of MOFs on the Carbon Dioxide Adsorption

임하늘, 임하늘, 고낙은, 최상범, 방남세, 김자헌

숭실대 화학과

Two new isoreticular MOFs that contained different side groups on their organic linkers, Zn4O(NH2NDC)1(BTB)4/3 (1) and Zn4O(NO2NDC)1(BTB)4/3 (2) were produced. Compared to the un-functionalized MOF, Zn4O(NDC)1(BTB)4/3 (3), 1 and 2 had slightly decreased BET (P/Po : 0.02 ~ 0.08) surface areas, 4440 and 4250 m2/g, respectively. However, the CO2 sorption measurements indicated that a higher CO2 uptake was observed for both 1 and 2 compared to 3. Interestingly, 2, which contained electron-withdrawing groups, exhibited an enhanced CO2 storage capacity over 1, which was decorated with electron-donating groups. The preparation, crystal structures, and various porosity properties of the isoreticular MOFs were examined with respect to the pore functionalization.

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Synthesis and Characterization of Nanohybrid Materials with Highly Crystalline Colloidal SnO_2 Nanoparticles and Exfoliated two dimensional MoO_3 Nanosheets

심은하, 고지은, 정현

동국대 화학과

To fabricate a novel mesoporous nanohybrid structure, the exfoliated MoO_3 nanosheets in aqueous solution were reassembled in the presence of surface modified SnO_2 nanoparticles. Two-dimensional nanosheets of orthorhombic MoO_3, as the host layered materials, were prepared by using ion exchange lithiation in the presence of an external oxidizing agent. The guest species, highly crystalline colloidal SnO_2 nanoparticles, were obtained by thermal decomposition reaction of tin 2-ethylhexanoate in the presence of *n*-dodecylamine as surface capping agents. The obtained SnO_2 nanoparticles have a diameter of around 3 nm with rutile crystalline. To fabricate nanohybrids, the hydrophobic nature of SnO_2 nanoparticles was changed to hydrophilic one by grafting reaction of (3-aminopropyl)trimethoxysilane (APS) molecules. Finally, the nanohybrid materials were obtained by electrostatic reassembling route between negatively charged MoO_3 nanosheets and positively charged water soluble surface modified SnO_2 nanoparticles. X-ray diffraction (XRD), Transmission electron microscopy (TEM), Fourier transform infrared (FT-IR) spectroscopy, N_2 adsoption-desoption isotherms, Atomic force microscopy (AFM), Inductively coupled plasma (ICP) and Thermal analysis (TG) were carried out to study the hybridizing process and the porous structure of nanohybrids.

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Preparation of Ni Nanoparticles in MOF-5 (Ni@MOF-5s) and Their Application for Hydrogen Storage

심재웅, 박영관, 최상범, 서장미, 김자헌

숭실대 화학과

MOF-5 could be loaded with Ni-nanoparticles by reducing the included nickelocene precursors under an H2 atmosphere. Using the gas-phase method, three Ni@MOF-5 samples were prepared, and the Ni content was varied stepwise with loadings of ~27, ~40, and ~47 wt%. While the Ni nanoparticles that were present inside the MOF reduced the surface areas of the Ni@MOF-5s, they provided additional hydrogen storage sites. The high pressure sorption measurements indicated that the main hydrogen uptake corresponded to the chemisorption. These results implied that the MOFs could be used as supports for nanometer sized metal hydrides, and thus, new hybrid systems could be developed to improve hydrogen storage materials.

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γ-ray Radiation Induced Synthesis and Characterization of α-Cobalt Hydroxide Nanoparticles

권법진, *김상욱, *박정훈, 정현

*동국대 화학과 *한국원자력연구원 방사선생명공학연구부*

A novel synthetic route has been developed to prepare α-cobalt hydroxide with nanometer size. It was successfully synthesized by γ-ray irradiation under simple conditions, i.e., air atmosphere, withoutbase. Under γ-ray irradiation, it leads to the formation of layered cobalt hydroxynitrate compounds with small crystalline size, due to the generation of hydroxyl anion by way of radiolysis reaction of hydrated cobalt nitrate in isopropanol. The obtained α-cobalt hydroxide had a uniform 3D flowerlike shape composed of aggregates of flakes which are built from nanocrystalline plates. Structural and morphological characterizations were performed by using power X-ray diffraction (XRD), field emission scanning electron microscopy (FE-SEM), and high resolution transmission electron microscopy (HR-TEM). The component and thermal stability of the sample were respectively measured by Fourier transform infrared (FT-IR) spectroscopy, elemental analysis, and thermal analyses, including thermogravimetry (TG) and differential thermal analysis (DTA).

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Carbon Nanotubes as Vehicle for Paclitaxel: Enhanced Water-Solubility and Anticancer Effects

이연주, *K. E. Geckeler

*광주과학기술원 신소재공학과 *광주과학기술원 신소재공학과,나노바이오전자재료공학과, 의료시스템학제학부*

Paclitaxel is one of the important and effective anticancer drugs for the treatment of various types of cancers, although its hydrophobicity and insolubility in water became a big hurdle for its administration. In order to overcome these problems and to enhance the anti-cancer effect, a synthetic polyampholyte for the enhancement of the water- solubility and carbon nanotubes as a drug carrier were employed to form a water-soluble supramolecular complex. The formulated paclitaxel nanoparticles, mediated by a synthetic polyampholyte, was loaded onto the nanotube surface. The resulting complex was investigated was found to be dispersible in water and to show a clear anti-cancer effect on MCF-7 human breast cancer and NCI-H358 human lung cancer cell lines.

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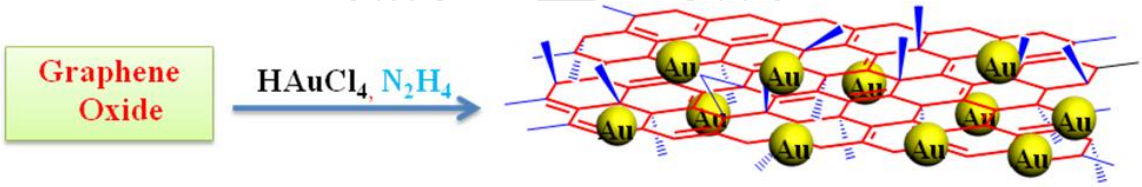
Au-Graphene Nanocomposites: Adsorption Properties of Au-Nanoparticls by Graphene-Concentration

문승진, 박경원, 정종화

경상대 화학과

Graphene oxide prepared using the Hummers method was centrifugation to yield aqueous dispersions of graphene oxide sheets. The desire to design metal-graphene nanocomposites assemblies has led us to explore a solution-based approach of chemical reduction of AuCl4-ions in graphene suspensions. The dependence of Au-particle formation on the graphene concentration. AFM, TEM and SEM analysis indicate that the gold nanoparticles are well dispersed on graphene sheets.



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Synthesis and Characterization of manganese oxide into pore of OMCs including heteroatom

문기영, 김지만

성균관대 화학과

Ordered mesoporous carbon (OMCs) have attracted considerable attention in various field of study due to high surface area. In particular, OMCs containing heteroatom(O, N, S, P, B and so on.) as the next generation energy storage device used in electrode materials are involved not only electrical double layer capacitor mechanism by high surface area but also operation of pseudo-capacitor by redox reactions of heteroatom. Thus, Manganese oxide was synthesized inside the pore system of host material OMCs containing heteroatom through a nano-replication method. The Mn/hetero-OMCs material thus obtained could be utilized excellent electrode of supercapapcitor, because it is exhibited simultaneously redox reaction and EDL reaction to obtain the greater capacitance.

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Graphene-Based Multifunctional Films with Tunable Physico-Chemical Properties

남보라, *이하진, *최원산

*충남대 분석과학기술대학원 *한국기초과학지원연구원 전주센터*

Since multifunctional freestanding films are very promising candidates for many potential applications in the fields of flexible electronics, photochromics, sensors, drug deliveries, and optical detection, many efforts have been devoted to fabrication and characterization of multifunctional films. In this paper, we report an advanced fabrication method for flexible, conducting, and transparent freestanding films involving encapsulated nanoparticles or nanoplates which confer characteristics of the films. These films were fabricated by combination of layer-by-layer (LbL) self-assembly and spin-assisted coating processes, which are simple, cheap, as well as commercially serviceable methods. A film composed of alternating layers of graphene-poly(allylamine hydrochloride) (G-PAH) and graphene-poly(styrene sulfonate) (G-PSS) was assembled on cellulose acetate (CA) as a sacrificial template. After depositing the desired number of layers, a thin CA was eliminated and then freestanding film was dethatched from quartz plate upon immersion in acetone. Buildup and formation processes of freestanding films were monitored by electron microscopy, atomic force microscopy, zeta-potential, and UV-vis spectroscopy. We believe that our fabrication techniques, the combination of spin-assisted coating and self-assembly, make the assembly process more efficient/easy and impart novel physical properties to the freestanding films.

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Nano-propping effect of residual silicas on reversible lithium storage over highly ordered mesoporous SnO2 materials

박귀옥, *문기영, *김지만

*성균관대 에너지과학과 *성균관대 화학과*

Highly ordered mesoporous SnO2 materials with residual silica species were successfully synthesized from a mesoporous silica template (SBA-15) via nano-replication and simple etching processes. A tin precursor, SnCl2•2H2O, was infiltrated spontaneously within the mesopores of the silica templates by melting the precursor at 353 K without using a solvent. After the heat-treatment of composite materials at 973 K under static air conditions, the controlled removal of silica templates using NaOH or HF solutions with different concentrations results in the successful preparation of mesoporous SnO2 materials, where the amounts of residual silica species are in the range 0.9–17.4 wt%. The residual silica species induce a nano-propping effect enabling the mesoporous SnO2 material (containing 6.0 wt% of silica species) to remain stable up to 973 K without any significant structural collapse. More importantly, the optimum amount of residual silica species (3.9–6.0 wt%) results in a dramatic reduction in capacity fading after prolonged charging–discharging cycles in Li-ion battery. The mesoporous SnO2 material with 3.9 wt% of silica species still exhibits a large capacity (about 600 mAh g-1) after the 30th cycle, which is probably because the residual silica species act as a physical barrier to suppress the aggregation of Sn clusters formed in the mesoporous SnO2 materials during the reversible lithium storage.

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Synthesis of Graphene/Polyaniline Nanocomposites and their Gas Sensing Properties

한승현, 신구, *L. Al-Mashat, *K. Kalantar-zadeh, *W. Wlodarski

*세종대 화학과 *RMIT University, Melbourne, Australia*

Graphene/polyaniline nano-composite has been developed through two template-free synthetic routes. Scanning Electron Microscopy (SEM) was used to characterize the resulting graphene/polyaniline nanocomposites yielded from the two syntheses. The solutions from these reactions were air-brushed on the surfaces of conductometric transducers. A comparison between the gas sensing performances of the two developed sensors is presented. It was found that the sensitive film based on the graphene/polyaniline nanocomposite directly synthesized from graphene has a sensitivity of ~ 20% towards 1% of hydrogen gas diluted in synthetic air. On the other hand the sensitive film based on the graphene/polyaniline nanocomposite synthesized from the reduction of graphene oxide/polyaniline has a sensitivity of only 4.43% towards the same concentration of hydrogen gas. All gas sensing measurements were conducted at room temperature. The developed sensors are promising for industrial applications.

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Polyaniline/MWNT Nanocomposite Based Hydrogen Sensor Operating at Room Temperature

한승현, 신구, *유봉영, **L. Al-Mashat, **K. Kalantar-zadeh, **W. Wlodarski

*세종대 화학과 *한양대 재료공학과 **RMIT University, Melbourne, Australia*

A nanocomposite of polyaniline (PANI) and multiwall carbon nanotubes (MWNT) has been synthesized and investigated as a sensing material for hydrogen gas at room temperature. The PANI/MWNT nanocomposite was prepared by in situ chemical polymerization. The nanomaterial characterization was conducted through Scanning Electron Microscopy (SEM) and Transmission Electron Microscopy (TEM). From these data it was concluded that the PANI formed conformal layer with thickness of approximately 7 nm aligned to the outer layer of the MWNT. A hydrogen sensor was developed by airbrushing the solution over the surface of heated conductometric transducer. The sensor was tested towards different concentrations of hydrogen gas at room temperature. At 1% of H_2 an increase in the sensing film resistance of 112 Ω as observed. The sensor maintained its stable baseline and repeatability during the testing period which makes it useful for commercialization purposes.

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Development of Chemical Sensor System for TNT

이웅희, 장현준, *김석찬, 유연규

*국민대 생명나노화학과 *국민대 화학과*

TNT 와 DNT 는 대표적인 폭발물이다. TNT 의 승화로 인해 발생하는 기체 TNT 를 검출하여 위험을 미연에 방지할 수 있는 Biosensor 를 만들기 위해, TNT 유도체인 3-(2,4,6-trinitrophenoxy)propan-1-aminium chloride 를 합성하였다. 3-(2,4,6-trinitrophenoxy)propan-1-aminium chloride 를 Biotine 나 SAMs 물질과 결합시켜 immobilize 하고, M13 phage 를 이용하여 TNT 에 특이적으로 결합하는 단백질을 찾아 Biosensor 를 만들고자 한다.

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Large area, directionally aligned single-walled carbon nanotube thin film by self-assembly technique

Najeeb.C.K, 창징보, 김재호

아주대 분자과학기술학과

Carbon nanotubes (CNTs) are among the most promising materials predicted to impact future nanotechnology owing to their exceptional structural and electronic properties. Aligned organization of nanotubes on a substrate is the primary requirement to exploit their unique electrical, optical and mechanical properties for their realistic potential applications. In our research, we employed surface modification of SWNTs with two different surfactants to meet the specific conditions for the self assembly of single-walled carbon nanotubes (SWNTs) in drop casted or spin coated films. The self assembly of nanomaterials from their surfactant dispersion is based on the shape, aspect ratio, surface charge and lateral capillary force during the drying process. First, we prepared SWNT dispersion with a biosurfactant sodiumdeoxycholate (SDC), which provided a rigid rod-like structure to the CNTs due to the presence of rigid steroid rings. Then, the dispersion was treated with an anionic surfactant, sodium dodecylbenzene sulfonate (SDBS) to generate negative charge on the CNT surface as well as to reduce surface tension of the medium. A large area aligned CNT film was obtained and the degree of alignment was varied with the ratio of SDC to SDBS in the solution.

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Highly sensitive ZnO UV Sensor

창징보, Najeeb.C.K, 김재호

아주대 분자과학기술학과

Heterojunctions with various compositions and interfaces have already demonstrated distinctive performances in nanodevice applications for optoelectronic technologies like light-emitting diodes, photovoltaics, and optical sensors. There has been great interest in UV sensor based on single walled carbon nanotube (SWNT)-zinc oxide (ZnO) heterojunctions because SWNTs can enhance UV photoresponse owning to high electron mobility. The SWNT-ZnO heterojunction film was fabricated by two step processes: first, a SWNT Langmuir-Blodgett (LB) film was deposited on an anodic aluminum oxide (AAO) template; and then, ZnO film was made by vacuum filtration of ZnO nanowire solution. The UV sensor based on combination of SWNT-ZnO demonstrated fast photoresponse. We also observed highly efficient photovoltaic effects in the SWNT-ZnO junctions when the device was illuminated by UV radiation.

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Nano-structured Films as a Novel Substrate for Cell Culture

김효섭, 강신범, 강원석, 김재호

아주대 분자과학기술학과

We fabricated a large area of monolayer silica nano-particle array on glass substrates for the cell growth by the Langmuir-Blodgett technique. A thin film of 300 nm sized mono-dispersed silica particles was constructed on the air-water interface and transferred onto a glass substrate. Chondrocytes were cultured on nano-structured substrates and bare glass for 8 days, respectively. The characterizations of chondrocytes on nano-structured substrate were conducted on 3rd and 6th day using confocal laser microscopy and with MTT assay for 8 days. The chondrocytes cultured on nano-structured substrate showed podia like spike and their size was larger than that formed on bare glass. The metabolic activity of chondrocytes on nano-structured substrate was lower than that on bare glass at early-stage, but it was recovered after 4 days.

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Electrodeposition of Hybrid Compound Consisting of TiO_2 and Polypyrrole

채원석, 한만소, 이소라, 김용국

대진대 화학과

An inorganic/organic hybrid compound consisted of TiO_2 and polypyrrole has been deposited by an electrochemcial anodic process in aqueous solution, and structurally characterized by SEM, XRD, IR, DSC and TG analysis. Moreover, the new properties of the hybrid compound are studied by the electrochemical method of cyclic voltammometry and chronoamperometry. Thses results show that the compound exhibits a composited feature of TiO_2 and polypyrrole. We propose that the hybrid compound as an electrode is applicable on an energy-storage and/or -conversion device.

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Exfoliation and Reassembling Route to Mesoporous Manganese Oxide Nanohybrids

이나라, 고지은, 정현

동국대 화학과

Novel mesoporous manganese oxide nanohybrids have been successfully synthesized by hybridization reaction of the exfoliated two-dimensional MnO_2 nanosheets and the surface modified colloidal Mn_3O_4 nanoparticles. The stable two-dimensional colloidal nanosheets, as a host materials, could be obtained by intercalating tetrabutylammonium cation into the birnessite(H)-type manganese oxide, $H_{0.13}MnO_2 \bullet 0.7H_2O$, and by successive exfoliating process in an aqueous solution. The guest species, colloidal monodispersed Mn_3O_4 nanoparticles, were prepared by thermal decomposition reaction of $Mn(acac)_2$ in the presence of oleylamine. To fabricate nanohybrids, the surface of obtained Mn_3O_4 nanoparticles was modified by 3-aminopropyltriethoxysilane molecules. Finally, the mesoporous manganese oxide materials were prepared by electrostatic reassembling route between negatively charged manganese oxide nanosheets and positively charged Mn_3O_4 nanoparticles. X-ray diffraction (XRD), N_2-adsoption-desoption isotherms, Transmission electron microscopy (TEM), Atomic force microscopy (AFM), Fourier transform infrared (FT-IR) spectroscopy and thermal analysis were carried out to study the hybridizing process and the porous structure of hybrid mesoporous manganese oxide.

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Development of SAW sensor device for detecting cartilage oligomeric matrix protein.

강신범, 김효섭, 김재호

아주대 분자과학기술학과

고감도로 타겟 물질을 검출하기 위해 프로브 물질을 센서 표면에 공유결합을 통해 고정화하는 기술을 개발하였다. 이러한 공유결합을 통한 방법은 기존의 물리흡착 방법에 비하여 세척 등과 같은 외부작용에 대하여 안정하며, 공유결합을 위하여 사용되는 유기재료에 의해서 단백질의 구조적 변성이 억제되는 효과가 있다. 이번 연구에서는 다양한 공유결합적 고정화 중에서 실질적인 제품 개발에 적합하도록 간단하면서도 재현성 있는 고정화 방법을 개발하고 이를 분석하였다.

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Monitored of Morphology of β-FeOOH, α-Fe_2O_3 and silica coated β-FeOOH, α-Fe_2O_3

유리, *피재환, 김유진

*한국세라믹기술원 엔지니어링세라믹센터 *한국세라믹기술원 도자기술센터*

The iron oxide has attracted wide at attention because they have been widely used as an electronic, magnetic materials and pigments. Especially, the α-Fe_2O_3 is a good candidate for replacement of red-pigments. However, they have the problem of forming aggregates at high temperature, which have a significant effect on the tonality of red color. Pigment must be thermally stable at the firing temperature. Also, β-FeOOH as well as α-Fe_2O_3 is transformed into hematite during heat treatment but heated of β-FeOOH to form micrometer-sized ill-shaped pieces. Thus, we suggest the use of core-shell type structure.(β-FeOOH@SiO_2, α-Fe_2O_3@SiO_2) The silica coated α-Fe_2O_3 nanoparticles retained their shapes after being heated at 1000℃. This study, morphology of β-FeOOH change during the heat treatment process was monitored as a function of temperature by TEM. Also, β-FeOOH@SiO_2, α-Fe_2O_3@SiO_2 were characterized by transmission electron microscopy (TEM), high temperature x-ray diffraction (HTX) and CIE L*a*b* colorimeter.

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Direct Preparation of 1-PSA Modified Graphene Nanosheets by Supercritical Fluidic Exfoliation and Their Electrochemical Application.

장지훈, 권영욱

성균관대 화학과

In situ surface modified/exfoliated graphene nanosheets (GNS) with different ratio of sulfonyl group on GNS surface were prepared by supercritical fluidic (SCF) reaction. Graphite flakes dispersed in the mixed solvent of distilled water and ethanol were exfoliated by SCF with various ratio of 1-pyrene sulfonic acid sodium salts (1-PSAs). The yield of GNS which confirmed by 2D band observation of Raman measurement shows above 60% of mono or double layered GNS. It is 4-times increased value as comparing with our previous results which are SCF exfoliated GNS without any modifying molecules. Also, as observing of D band difference between the pure GNS and the sulfonyl groups modified GNS, we confirmed that sulfonyl groups on GNS makes electron poor surface of GNS. In order to prove the absence of any other contaminants and show the well exfoliated GNS, XRD, IR, TEM and AFM measurements were done. Electrochemical Li-ions charging-discharging behavior of the sulfonyl groups modified GNS was carried out with a standard 3-electrode cell and compared with the graphite flakes. We obtained not only a larger capacitance for Li ions with the sulfonyl groups modified GNS than graphite flakes but confirmed a different way to charge and discharge Li ions.

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Design and Synthesis of Hetero-Structure Metal Nanoparticles for Optical Properties

양희승, *김유진, **정운룡

*한국세라믹기술원 에너지반도체센터 *한국세라믹기술원 엔지니어링세라믹센터 **연세대 신소재공학과*

Inorganic coating of metal nanoparticles has attracted wide at attention due to their chemical stability and optical properties. Especially, control of morphology in titanium oxide coated metal nanoparticles is important factor for efficient electron transfer in solar cell applications. In this work, we proposed core-shell type TiO_2/SiO_2 Hetero-structure nanoparticles coating metal nanoparticles. Gold nano particles were coated with TiO_2/SiO_2 as a precursor titanium isopropoxide (TTIP) and tetraorthosilicate (TEOS) by micro-emulsion method. The prepared TiO_2/SiO_2 coated nanoparticles were structurally characterized by X-ray powder diffraction (XRD), transmission electron microscopy (TEM) and spectroscopic analysis for their optical properties.

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Neutron diffraction analysis for Li-ion conductors, $Li_{5+x}La_3Zr_xTa_{2-x}O_{12}$ (x = 0 - 1.5)

김성철, 김승주

아주대 에너지시스템학부

Solid state lithium ion conductors, $Li_{5+x}La_3Zr_xTa_{2-x}O_{12}$ (x = 0 - 1.5) were synthesized by conventional solid state reaction. The structures of compounds were characterized by Rietveld refinement using the powder neutron diffraction data. All the compounds exhibit a garnet-type structure with cubic symmetry (space group: *Ia-3d*). The lattice parameter of $Li_{5+x}La_3Zr_xTa_{2-x}O_{12}$ increase as increase the zirconium content (a=12.83 Å for $Li_5La_3Ta_2O_{12}$, a=12.96 Å for $Li_{6.5}La_3Zr_{1.5}Ta_{0.5}O_{12}$).

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Octahedral tilting and anion ordering in oxynitride perovskites $SrTaO_2N$, $CaTaO_2N$, and $LaTaON_2$

이은혜, *김영일

*영남대 이과대학/화학과 *영남대 화학과*

Crystal structures of mixed anion perovskites, $BaTaO_2N$, $SrTaO_2N$, $CaTaO_2N$, and $LaTaON_2$ are examined by Rietveld refinements of neutron diffraction patterns collected at 300 K. With the size reduction of dodecahedral cation, from Ba^{+2} to Sr^{+2} to Ca^{+2} to La^{+3}, octahedral tilting becomes more pronounced, resulting in cubic (*Pm*3*m*), tetragonal (*I*4/*mcm*), orthorhombic (*Pnma*), and monoclinic (*C*2/*m*) systems, respectively. The latter three phases with lower symmetries contain multiple anion sites, to open chances of O/N ordering. Present investigation reveals that the anion ordering in those oxynitride perovskites is promoted by the use of flux additives in the sample preparation stage. Distinct anion ordering behaviors among $SrTaO_2N$, $CaTaO_2N$, and $LaTaON_2$ are discussed in terms of bond valence sum rationale.

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Various Nanotube/Nanowire Arrays with CdS and ZnSe outerlayers for Photoelectrochemical hydrogen production

손용재, 장동명, 명윤, 성태광, 조용재, 김한성, 박정희

고려대 소재화학과

High-density TiO2 nanotube arrays were synthesized using electrochemical method, and CuO nanowire array was synthesized using thermal oxidation of Cu foils. Their diameter was controlled using the growth condition. The CdS and ZnSe layers were uniformly deposited on the pre-grown TiO2 nanotubes (anatase) and CuO nanowires, using vapor transport method. The thickness of the CdS shell was uniformly controlled to be 10-50 nm. The CdS and ZnSe shell layers consisted of a number of single-crystalline domains whose wurtzite [001] direction aligned along the wire axis. The thicker outerlayer results in a higher value of photoconversion efficiency. As the thickness of shell in the nancables increases, a hydrogen generation rate under visible light irradiation increases.

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Selectively aligning twin-free epitaxial Pd nanowire arrays: parallels, squares, and verticals

유영동, 이효반, *안재평, 김봉수

*KAIST 화학과 *KIST 산업화지원센터*

We report that twin-free single-crystalline Pd nanowire arrays grow epitaxially in a selected direction on a substrate. Parallelly aligned Pd nanowires are synthesized on a $SrTiO_3$ (110) substrate in a very high density. On a $SrTiO_3$ (001) substrate Pd nanowires grow horizontally in two perpendicular directions. We synthesize vertical Pd nanowires instead of horizontal nanowires when c-cut sapphire is employed as a substrate. We reveal that the nanowires grow from the seeds and the atomic structure of the substrate surface determines the geometry and orientation of seeds, which in turn direct the growth patterns of the nanowires. The interface energy between the nanowire material and the substrate is also critical in determining the nanowire growth pattern. Polarization-dependent localized surface plasmon resonance of as-synthesized epitaxial Pd nanowire arrays is investigated for application as a plasmonic platform.

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Steering epitaxial alignment of noble metal nanowire arrays by atom flux change

유영동, *안재평, 이효철, 김봉수

*KAIST 화학과 *KIST 산업화지원센터*

We have synthesized epitaxial Au, Pd, and AuPd nanowire arrays in vertical or horizontal alignment on a c-cut sapphire substrate. We show that the vertical and horizontal nanowire arrays grow from half-octahedral seeds by the correlations of the geometry and orientation of seed crystals with those of as-grown nanowires. The alignment of nanowires can be steered by changing the atom flux. At low atom deposition flux vertical nanowires grow, while at high atom flux horizontal nanowires grow. Similar vertical/horizontal epitaxial growth is also demonstrated on $SrTiO_3$ substrates. This orientation-steering mechanism is visualized by molecular dynamics simulations.

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Gold Nanoparticles Supported on a Superparamagnetic Silica Microsphere

한승현, 허남회

서강대 화학과

We report the synthesis and catalytic activity of Au nanoparticles (NPs) anchored on a superparamagnetic mesoporous silica microsphere, denoted as Au-CoFe2O4@SiO2. The Au NPs are immobilized on the surface of a mesoporous silica microsphere using urea as a linker molecule. The Au-CoFe2O4@SiO2 catalyst was completely characterized by XRD, SEM, TEM, and magnetization measurements. Using the Au-CoFe2O4@SiO2 catalyst, we carried out catalytic reduction of 4-nitrophenol in which the products were carefully characterized by UV-visible spectrometer and NMR. Even with small amount of NaBH4, the reduction reaction proceeds smoothly at room temperature. The Au-CoFe2O4@SiO2 catalyst is very stable and is easily recovered by a magnet. The activity for the hydrogenation reaction with the used catalyst was not noticeably changed, thus showing good potential as a recyclable catalyst.

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Filling the pore dimension gap of nanotemplates : Synthesis of Mesoporous Silica Thin Films with 10-20 nm pores

이기림, 권영욱

성균관대 화학과

Nanoporous thin films are finding ever increasing applications in diverse fields such as media for adsorption or immobilization of biomolecules such as enzymes, templates for the synthesis of nanostructured materials including quantum dot arrays, drug delivery systems, and sensors. At present, anodized aluminum oxide (AAO) and self-organized block copolymer films have been widely explored. In addition, our group and a few others have been working on developing mesoporous thin films. The typical pore dimensions of AAO, block copolymer, and mesoporous thin films are > 30 nm, 20-40 nm, and 2-10 nm, respectively. These pores sizes leave a gap in the range of 10-20 nm. In this study, we synthesized mesoporous silica films with 10-20 nm pores to fill the pore dimension gap. In order to increase the size of the hydrophobic core of the self-assemble which can be an important size regime for the above mentioned applications structures, we introduced swelling agents such as 1,3,5-trimethylbenzene (TMB) and poly(propylene oxide) (PPO). We used various molar ratios of surfactant/swelling agents to induce the swelling of surfactant micelles. The swelling process eventually leads to the control of pore diameter the resultant mesoporous silica thin films. This also enabled us to control the pore structures including the cubic and hexagonal structures. X-ray diffraction (XRD), scanning electron microscopy (SEM) and transmission electron microscopy (TEM) techniques were used to observe the pore diameter, silica wall thickness, and the structure of the mesoporous thin films.

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Preparation of Multimodal Porous Magnetic Mesoporous Silicas by Hydrogen Reduction Process

이지호, *장정호, 박상언

*인하대 화학과 *요업기술원 바이오IT융합센터*

Multimodal porous structure of magnetic mesoporous silicas was prepared using the hydrogen reduction process. Mesoporous silicas were combined with iron(II) chloride tetrahydrate for initiating magnetizing process, followed by reduction in H_2 media for etching. We present to results of the magnetism and multimodal porous structure from the temperature (400 ^oC to 800 ^oC) effect in the hydrogen reduction process. The multimodal pore sizes magnetic mesoporous silicas were characterized by various state-of-the-art techniques, such as SAXS, WAXS, FE-SEM, TEM, FT-IR, SQUID and nitrogen adsorption. We confirmed multimodal porous structure of magnetic mesoporous silicas has superparamagnetic and variou pores size (10 nm to 100 nm) in accordance with temperature in the hydrogen reduction process.

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Colloidal phosphors of layered rare-earth hydroxides

배정수, 이병일, 변송호

경희대 화학과

Layered rare-earth hydroxynitrates, $RE_2(OH)_5NO_3 \bullet nH_2O$ where RE = Eu, Gd, Tb and Er were synthesized by using a hydrothermal reaction under a controlled pH condition. Formation of single phase was confirmed by X-ray diffraction which showed characteristic strong (0 0 *l*) reflections of layered material. The chemical compositions of $RE_2(OH)_5NO_3 \bullet nH_2O$ were determined by inductively coupled plasma(ICP), thermogravimetric(TG), element analysis(EA). Existence of nitrate anions in the interlayer space was demonstrated from specific peaks which stand for N-O vibration mode in Fourier transform infrared(FT-IR) spectra. Exfoliation was accomplished in formamide and colloidal suspensions of layered compounds were obtained through ultrasonic process. The thickness and size of dispersed nanosheets in resulting colloidal suspensions were measured by atomic force spectroscopy(AFM). When irradiated with 365nm UV, the resulting transparent colloidal solution of fomamide containing europium and terbium hydroxide nanosheets yielded typical red and green emissions, respectively, which are visible to the naked eye.

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Immobilization of polyoxomolybdates on the layered gadolinium hydroxide nanosheets by self-assembly method

이병일, 정희진, 변송호

경희대 화학과

Novel self-assembly of layered gadolinium hydroxide nanosheets and polyoxomolybdates was achieved at pH_4^{2-}) can be converted to heptamolybdate($Mo_7O_{24}^{6-}$, called polyoxomolybdate) at pH 4~5. The layered hydroxocations delaminated from layered gadolinium hydroxides(LGdH) were easily assembled with polyoxometalate anions to micrometer sized aggregates by layer-by-layer stacking mode. The results of X-ray diffraction(XRD) and field emission scanning electron microscopy(FE-SEM) showed that resulting samples are single phase and have a heirarchical rose-like superstructures. Existence of $Mo_7O_{24}^{6-}$ in the interlayer was confirmed by infrared(IR) and Raman spectroscopy. The contents of molybdenum and gadolinium were determined by inductively coupled plasma(ICP). The rose-like superstructure endured up to ~300℃ and its self-assembly behavior was irreversible despite the solution pH was increased to ~10.

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Epitaxial growth of ZnO nanowires on vertical Au nanowires

김민정, *유영동, *김봉수

*KAIST 나노과학기술대학원 *KAIST 화학과*

Hierarchical heterostructures are useful for the realization of 3D multicomponent functional nanodevices since the cores and branches of these nanostructures are composed of different materials. Specially, metal-semiconductor heterostructures have attracted great attention recently because of their unique optical, electrical, and catalytic properties and potential applications. Hierarchical nanostructures with Au backbone and ZnO branches are successfully prepared by a simple chemical deposition without using any catalysts or capping reagents.Vertical Au nanowires were grown on SrTiO_3(110) with high density because of their good lattice match. A secondary growth process was carried out for ZnO branchs growth on primary Au nanowires. The ZnO branches are perpendicular to the central axis, which shows six-fold symmetry.

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Transparent and Conducting Thin Films Using Layer-by-Layer Assembly of Negatively and Positively Charged Reduced Graphene Oxides

이동욱, 이지숙, 신현석

울산과학기술대 에너지공학부

Graphene, as a single-atom-thick sheet of hexagonally sp2-bonded carbon atoms, is a rapidly rising star in materials science and condensed matter physics. This two dimensional material exhibits exceptionally unique electronic, mechanical and thermal properties. However, in order to make transparent electrode it is difficult to pile up the graphene layers because of hydrophobic nature. Herein, we synthesized stable suspension of positively and negatively charged reduced graphene oxide, respectively. By exploiting the electrostatic interactions between these oppositely charged reduced graphene oxide suspensions, we made a thin film of multilayered graphene nanosheets using layer-by-layer assembly methods. The assembled graphene multilayer thin film exhibits an excellent electrical conductivity with a high optical transmittance. Furthermore, we compare the thin film fabricated by layer-by-layer assembly of reduced graphene oxides with that of graphene oxides. Lastly, we show a light-emitting diode based on these assembled graphene multilayer as a transparent and conducting electrode.

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Mesoporous Silica Thin Film with Ordered Lamellar Structure for Low-k Material Application

박정규, 이기림, 권영욱

성균관대 화학과

We report the synthesis of silica thin films with an unusual structure and unusual physical properties arising from the structure. The thin films were synthesized by sol-gel chemistry with a neutral surfactant as the structure-directing agent followed by controlled aging and calcination. The thin film deposited by spin-coating process. The X-ray diffraction (XRD), transmission electron microscopy (TEM), scanning electron microscopy (SEM) data all indicated that these films had lamellar structures with modulated silica density with alternating high density layers and low density layers. Nanoindentation measurement data on these films produced 1-2 GPa for the hardness and 20-25 GPa for the Young's modulus, which are unusually high for pure silica films. Typical sol-gel silica films have 0.2-0.3 GPa of hardness and 2-10 GPa of Young's modulus. Also we modified the surface of films to be hydrophobic by HMDS(Hexamethyl disilazane) treatment. In this presentation, the formation mechanism and details of the characterization data of our silica films will be presented.

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Three-Dimensional Structure of Twinned and Zigzagged One-Dimensional Nanostructures Using Electron Tomography

김한성, 명윤, 조용재, 장동명, 정찬수, 박정희, *안재평

*고려대 소재화학과 *KIST 산업화지원센터*

Electron tomography and high-resolution transmission electron microscopy were used to characterize the unique 3-dimensional (3D) structures of twinned Zn_3P_2 (tetragonal) and InAs (zinc blende) nanowires synthesized by the vapor transport method. The Zn_3P_2 nanowires adopt a unique superlattice structure that consists of twinned octahedral slice segments having alternating orientations along the axial [111] direction of a pseudo cubic unit cell. The apices of the octahedral slice segment are indexed as six equivalent directions at the [111] zone axis. At each 30 degrees turn, the straight and zigzagged morphologies appear repeatedly at the and zone axes, respectively. The 3D structure of the twinned Zn_3P_2 nanowires is virtually the same as that of the twinned InAs nanowires. In addition, we analyzed the 3D structure of zigzagged CdO (rock salt) nanowires and found that they include hexahedral segments, whose six apices are matched to the directions, linked along the [111] axial direction. We also analyzed the unique 3D structure of rutile TiO_2 (tetragonal) nanobelts; at each 90 degree turn, the straight morphology appears repeatedly, while the in-between twisted form appears at the [011] zone axis. We suggest that the TiO_2 nanobelts consist of twinned octahedral slices whose six apices are indexed by the / directions with the axial [010] direction.

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Exfoliation-Reassembling Synthesis of Intercalative Transition Metal Oxide-Graphene Nanohybrid

김인영, *김태우, **황성주

*이화여대 나노과학부 *이화여대 지능형 나노바이오소재 연구센터 **이화여대 화학·나노과학과*

A new intercalative nanohybrid of chromium oxide-graphene was successfully synthesized via exfoliation-reassembling route. The intercalative hybridization of the exfoliated graphene nanosheets with chromia nanoclusters was achieved by an electrostatic attraction between these oppositely charged species. According to powder X-ray diffraction and transmission electron microscopy analyses, nanosized chromia nanoclusters (ca. 6.4 Å in diameter) are intercalated in-between two-dimensional graphene layers. Cr K-edge X-ray absorption near edge structure spectroscopy clearly demonstrated that the heat treatment of the as-prepared nanohybrid at elevated temperatures induces a transformation from chromia nanocluster to nanosized chromium oxide. Evolutions of optical property upon the hybridization and post-calcination were evidenced by diffuse reflectance UV-vis spectroscopy, confirming the hybridization of chromia and the following phase transformation of the guest species. To the best of our knowledge, this is the first example of pure intercalation compound prepared by the reassembling between exfoliated graphene nanosheets and metal oxide nanoclusters.

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Preparation and Evaluation of Antimicrobial and Biodegradable PGLA Sutures

이혜선, *장정호

*연세대 신소재공학과 *요업기술원 바이오IT융합센터*

This work demonstrates the development of novel antimicrobial and biodegradable suture coated by natural extract from grape fruit. The natural extract is loaded to PLGA suture and their optimum conditions are determined for soaking time, loaded volume, and releasing time. Furthermore, the evaluation of antibacterial effect was achieved by Staphylococuus aureus as a function of used amounts and released time. The cell growth was also calculated for several days through 2 month. The physicochemical properties of antimicrobial and biodegradable PLGA suture are demonstrated.

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Highly selective protein separation with cooperative functionalized magnetic nanoparticles.

안치영, *장정호, 김웅

*고려대 신소재공학부 *요업기술원 바이오IT융합센터*

This work reported the development of the high efficient protein separation process with molecularly assembled silica coated magnetic nanoparticles as the cooperative functional groups. The surface modification was performed with functionalized organosilanes such as thiol-, disulfide-, and dodecyl-groups. The silica coated magnetic nanoparticles were directly produced by the sol - gel reaction of the tetraethyl orthosilicate precursor. The protein separation with cooperative functionalized magnetic nanoparticles was achieved for model protein such as bovine serum albumin (BSA) and Lysozyme (LSZ) at different pH conditions. The work on using silica coated magnetic nanoparticles for protein separation have the advantages such as easy preparation , easy handling and extensive potential of biotechnology application.

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Synthesis and Pillaring of Multilamellar MFI Zeolite Nanosheets with a Single-Unit-Cell Thickness

나경수, 박우진, 유룡

KAIST 화학과

Single-unit-cell thick MFI zeolite nanosheets have been synthesized via cooperative assembly between silica and an organic surfactant containing a diquaternary ammonium group, i.e., $C_{22}H_{45}$-$N^+(CH_3)_2$-C_6H_{12}-$N^+(CH_3)_2$-C_6H_{13}. Hydrophobic interactions between the surfactant tails allow the zeolite nanolayers to be further assembled into an ordered multilamellar mesostructure. In this presentation, synthesis conditions, effects of Al incorporation, control of interlamellar spacings, and the assembly process into multilamellar MFI zeolite nanosheets are discussed. We also demonstrate that silica pillaring between the adjacent 2-nm-thick MFI layers in the multilamellar mesostructure can develop a hierarchically ordered mesoporous/microporous zeolite, exhibiting small angle X-ray diffraction peaks up to the fourth-order reflections. This is the first ordered material with 3D-structured zeolite framework. Interestingly, Ar adsorption and transmission electron microscopic analyses indicate that the pillars are highly likely to be built with an MFI framework.

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Immobilization of DNA and Polyoxometallate Anions in the Interlayer Space of Surface-Modified Layered Metal Oxide

김태우, *김인영, **황성주

*이화여대 지능형 나노바이오소재 연구센터 *이화여대 나노과학부 **이화여대 화학·나노과학과*

In this study, we have developed a new methodology of surface modification-exfoliation-reassembling for the intercalative hybridization of anionic species like deoxyribonucleic acid (DNA) and polyoxometallate with layered metal oxide having intrinsic negative layer charge. For the surface modification, first we expanded the interlayer distance of layered titanate by the intercalation of octylamine. Then, 3-aminopropyltriethoxysilane (APS) was anchored onto the interlayer surface of layered titanate by condensation reaction between hydroxyl groups on the surface of the titanate sheet and ethoxy groups of APS. The surface modification of layered titanate by APS-anchoring was confirmed by (^{29}Si magic angle spinning-nuclear magnetic resonance (^{29}Si MAS-NMR) and FT-IR spectroscopy showing the formation of Si-O-Ti bond. According to zeta potential measurement, the surface-modified layered titanate shows positive surface charge at pH < 6, which contrasts with the unmodified titanate nanosheet having zero surface charge at the same pH region. With the help of surface modification, we were successful in intercalating biomolecular DNA anions as well as inorganic polyoxovanadate anions into the layered titanate. The crystal structure and chemical bonding nature of the anion-intercalated titanates was systematically investigated with combination of diverse diffraction, microscopic, and spectroscopic tools. In particular, the immobilization of DNA in the titanate lattice was confirmed by FT-IR spectroscopy and electrophoresis.

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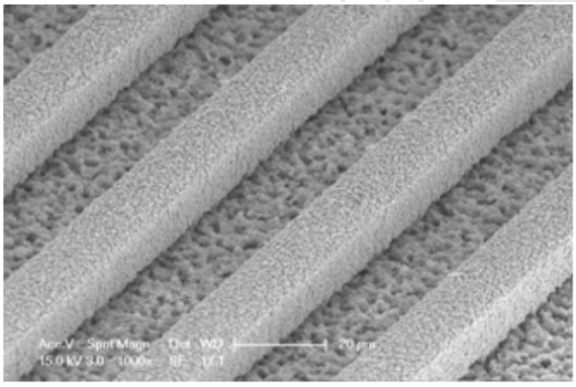
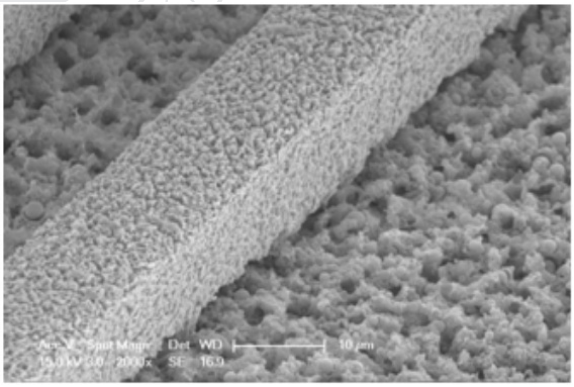
Development of Organic Acid Type Soft Etching(Micro Etching) Solution for Manufacture Process of Printed Circuit Board

이진규, *이학준

*한양대 바이오나노학과 *한양대 응용화학과*

In the manufacture process of Printed Circuit Board(PCB), Soft Etching(Micro Etching) increases the adhesive strength between copper surface and Photo Solder Resists Ink(PSR Ink). Sufuric acid-hydrogen peroxide solution was widely used previously. However, sufuric acid-hydrogen peroxide solution has limits in the process under 50 ㎛ owing to loss of circuit width. We developed the new efficient process for soft etching with organic acid solution.





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High-Resolution SEM Investigation and Monte Carlo Simulation on Mesopore Generation by Organosilane Surfactant during LTA Zeolite Crystallization

조강희, *Shunsuke Asahina, **Michael W Anderson, ***Osamu Terasaki, 유룡

*KAIST 화학과 *JEOL(Europe) **School of Chemistry, The University of Manchester ***Structural Chemistry, Arrhenius Laboratory, Stockholm University*

The crystallization of LTA zeolite under a hydrothermal synthesis condition containing a quaternary ammonium-type organosilane surfactant was studied with high-resolution scanning electron microscopy (HRSEM) and Monte Carlo simulation of the crystal growth. The synthesis products, collected at various crystallization times, were investigated by high-resolution scanning electron microscopy (HRSEM) as synthesized and also after cross-sectioning the crystal with an argon ion beam. The HRSEM imaging experiment revealed the presence of fully disordered network of mesopores as penetrating throughout the entire volume of the microporous zeolite crystal. Despite the penetrating mesopores, the microporous zeolite particles obtained at a low concentration of the organosilane surfactant still exhibited a truncated cubic morphology like single crystals. The outline of the zeolite particle became progressively rounded as the surfactant concentration and thereby the mesoporosity were increased. Except at highly basic conditions, the mesoporous structure in the zeolite crystal has been well maintained against the crystal-ripening process for 6 d under the given synthetic condition. These results support that the organosilane surfactant micelles became quite homogeneously incorporated inside the zeolite crystal during the crystal formation, certainly as a mesopore generator. Data from Monte Carlo simulation agreed with these experimental results.

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New Visible Light-Driven Photocatalysts for Hydrogen Production: CdS Quantum Dot-Tungsten Oxide Nanohybrids

김효나, *김태우, **김인영, ***황성주

*이화여대 화학·나노과학과 *이화여대 지능형 나노바이오소재 연구센터 **이화여대 나노과학부 ***이화여대 화학·나노과학과*

We were successful in synthesizing novel CdS quantum dot (QD)-tungsten oxide nanohybrids in terms of electrostatic attraction between the two components. First, we prepared amine-modified CdS QD having positive surface charge by one-pot soft-chemical reaction. Then the obtained suspension of well-disperse amine-modified CdS QD was added to aqueous solution of polyoxotungstate anions at the constant pH of 4, resulting in the formation of CdS QD-tungsten oxide nanohybrid. According to UV-vis spectroscopy, CdS QD-tungsten oxide nanohybrid showed a distinct change of optical property reflecting the presence of electric coupling between the two components. Also, it was found that the lifetime-decay of exited electrons in QD (at ex. 400 nm) was prolonged after hybridization with tungsten oxide. Furthermore, the photostability of the CdS QDs was significantly improved by the electronic coupling with tungsten oxide. More importantly, the as-prepared and calcined nanohybrids show very promising photocatalytic activity against the visible light-induced water splitting for hydrogen production.

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Al/PEDOT:PSS/Al 저항 메모리 소자의 메커니즘 규명

김종윤, 윤태현, *최성율

*한양대 화학과 *한국전자통신연구원 나노전자소자팀*

본 연구에서는 Al/PEDOT:PSS/Al 메모리의 이극성 저항변화특성의 메커니즘을 밝히기 위해 상부전극을 각각 Al 과 Au 를 증착하여 비교함으로서 상부 계면층의 형성이 중요한 요인임을 증명하였다. I-V 특성에 의해 Al 소자에서는 이극성 저항변화 특성이, Au 상부 전극에서는 permanent breakdown 현상이 확인되었으며, Al 소자에서의 전류이동모델은 I-V double-log plot 해석에 의해 SCLC 모델로 기술될 수 있었다. 저항변화 메커니즘을 분석하기 위하여 고분해능 투과전자현미경(HRTEM) 과 in situ X-선 광전자 분광기(In-situ XPS) 방법이 사용하였으며, Al 과 Au 상부전극 소자의 단면을 HRTEM 관찰 결과 Al 상부전극은 활성층과의 계면에서 새롭게 형성된 상부계면층이 관찰되었으나 Au 상부전극에서는 뚜렷한 계면층이 발견되지 않았다. 이러한 HRTEM 관찰 결과는 상부전극의 Al 과 활성층의 PSS-chain 에 있는 SO3-작용기의 O 와 S 가 Al 과 반응하면서 Al-O 와 Al-S 가 되지만 Au 상부전극의 경우 활성층과의 반응이 없기 때문임을 In-situ XPS 측정으로 확인할 수 있었다. 이러한 관찰 결과를 근거로 산소와의 반응성이 강한 Al 금속전극이 PEDOT:PSS 유기층과의 반응에 의해 생긴 전하 트랩 사이트들이 저항변화의 요인임을 확인하였다.

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Cucurbit[6]uril: Organic Molecular Porous Material for Proton Conductivity

김현욱, 서경원, 김용휘, 김기문

포항공과대 지능초분자연구단, 화학과, 첨단재료과학부 (WCU)

Search for new materials for high proton conductivity has been a hot issue in applications of fuel cell membranes. An organic molecular porous material based on cucurbituril (CB[6]) including water and HCl molecules in the channels may have potential as a proton exchange membrane. Here we present the proton conductivity of CB[6] measured by two-probe method at various temperatures. The proton conductivity of CB[6] is 1.1×10^{-4} at room temperature, which is comparable to those of other porous materials with well-defined pore size. The conductivity increases with increasing temperature up to 80 °C and the activation energy estimated by the Arrhenius equation is 0.37 eV. In order to directly confirm the proton transfer along the channels, we measured *I-V* curves using a single-crystal aligned along the *c* axis on a nano-device. Details of the work will be presented.

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The computational investigation on the CO_2 adsorption onto the B-doped BNNT(8,0) sidewall

최희철, 박영춘, 이윤섭

KAIST 화학과

The rapid increase in the level of anthropogenic carbon dioxide (CO_2) is a matter of great concern. While discussions have begun on means to reduce CO_2 emissions, it is apparent that atmospheric CO_2 concentrations will continue to monotonically increase due to fossil fuel consumption. Therefore, the capture and storage of CO_2 is very important in environmental, biological, and industrial processes. Recent experiment showed that carbon and boron-nitride nanotubes (CNT and BNNT) can act as chemical sensors for detecting certain gaseous molecules such as NH_3, NO_2, and O_2. Unfortunately, the intrinsic stability of CO_2 makes its sensing by nanotubes unsuccessful due to the rather weak adsorption energy on the tube surface. In this work, we study the CO_2 adsorption on the B-doped zigzag (8,0) single-walled BNNT to explore the possibility of B-doped BNNTs as potential materials for CO_2-capture by ONIOM calculations, which consist of DFT methods in the high computational part and AM1 in the low part. The appreciable adsorption energies and CO_2-adsorption mechanisms indicate that B-doped BNNTs can serve as efficient materials for CO_2-capture and storage.

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Investigations of the Growth Mechanism/Optical Properties of Hexagonal Au Nanoplates

홍순창, 이두리, 김수진, *장호영, 박성호

*성균관대 화학과 *성균관대 에너지과학과*

Hexagonal gold nanoplates were synthesized by the seed-mediated etching and growth process. Triangular prisms(seed) were etched by Au3+ ions and gold ions was reduced by dropwise addition of ascorbic acid. As a result, triangular prisms grow into hexagonal plates. Furthermore, we can tailor the thickness of Au plates between 20nm to 170nm. Each optical property of gold nanoplates was characterized by UV-vis-NIR spectroscopy and transmission electron microscopy(TEM) technique. The optical properties of them were calculated using the discrete dipole approximation(DDA) and compared with the experimental measurements.

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Phase Transfer of Gold Nanoparticles from Aqueous to Organic Medium

백효진, 김현정, *박연주, **장민선, 박성호

*성균관대 화학과 *성균관대 에너지과학과 **성균관대 물리.화학융합협동과정*

Citrate-stabilized sphere-type gold nanoparticles were prepared in aqueous phase and transferred to organic phase by alkanethiol. We also transferred the rod-type and plate-type gold nanoparticles to organic phase. The particles could be easily phase-transferred into organic solvent, redispersed in a variety of solvent such as benzene, hexane, cyclohexane. The gold nanoparticles were stable for months in the organic solvent.

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Synthesis of Vertically Aligned Hollow Platinum Nanotube

LIULICHUN, *유상훈, **조상현, *이상아, ***조성환, *박성호

*성균관대 화학 *성균관대 화학과 **성균관대 에너지과학과 ***성균관대 에너지과학학과*

We report here on a methodology for synthesizing vertical arrays of hollow Pt nanotubes with single crystalline nanoflakes. Initially, single component Ni nanorods were fabricated with the aid of AAO templates and electrochemical deposition. When the resulting Ni nanorods were immersed in Pt ion-containing aqueous solution, the Ni metal dissolved into Ni2+ ions through spontaneous galvanic replacement with Pt ions. However, the direct replacement between Ni nanorods and Pt ions led to an irregular architecture in the resulting Pt deposition. Instead, a pitting corrosion pretreatment of the Ni nanorods produced nucleation sites for the replacement with Pt ions. This step was critical for accelerating the interfacial replacement reaction rate and the formation of the regular Pt nanotubes with sultrathin superficial nanoflakes. We found that the Kirkendall effect was operative in the Pt nanotube formation.

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Synthesis and Characterization of Polyelectrolytes-Manganese Oxide Heterostructures

이경민, *김태우, **김인영, ***황성주

*이화여대 화학나노과학과 *이화여대 지능형 나노바이오소재 연구센터 **이화여대 나노과학부 ***이화여대 화학·나노과학과*

Various organic polyelectrolytes of poly(diallymethyl ammonium chloride), polyethyleneimine, poly(allylamine hydrochloride), and poly(4-vinylpyridine) were intercalated into the layered manganese oxide for the first time. These heterostructured compounds could be synthesized *via* self-assembly reactions between negatively charged manganate nanosheets and positively charged polyelectrolytes. According to powder X-ray diffraction analysis, all the present materials show equally spaced (00*l*) Bragg reflections at low angle region, indicating the formation of single phase intercalation compounds. Their basal spacings (ca. d_{001} = 1~1.50 nm) are strongly dependent on the dimension of the guest polyelecterolytes. The immobilization of polyelectrolytes in the manganate lattice was confirmed by the results of FT-IR analysis showing characteristic absorption peaks of polyelectrolytes corresponding to the stretching/bending modes of $-CH_2-$ and -CN-. The present heterostructured materials were applied as cathode materials for lithium ion secondary batteries. Based on these results, we will discuss the effect of polyelectrolyte-intercalation on the electrochemical activity of layered manganese oxide in detail.

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발표종류: 포스터, 발표일시: 금 15:00~17:00

Synthesis and characterization of green dyes for printable color filter suitable for LED BLU

김세훈, *김재필

*서울대 공과대 재료공학부 *서울대 재료공학부*

최근 LCD 의 백라이트는 저전력형이 LED 등의 백색광원을 사용하는 추세로서 LED 광원에 대응하는 칼라필터가 별도로 필요하다. 현재는 안료형의 LED 대응 칼라필터를 사용하고 있으나 고색대비형의 염료형 또는 안료-염료 하이브리드형의 칼라필터 개발이 진행 중에 있다. 현재 LCD 기술의 진행방향을 살펴볼 때 저전력화, 제조공정의 단순화, 고색재현율, 고명암비 구현등이 핵심 요구사항으로서, 본 연구개발에서는 저전력형 LED 백라이트에 대응할 수 있으며 동시에 ink-jet printing 을 이용하여 칼라필터를 제조할 수 있는 printable 염료형의 칼라필터용 잉크를 개발하고자 한다.

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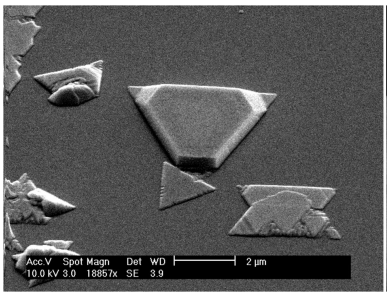
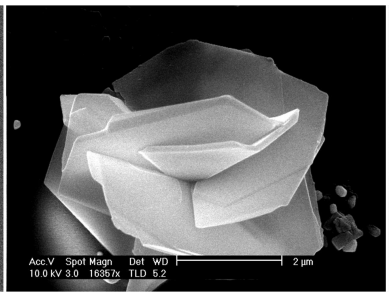
The role of O_2 flow rate for synthesis of NiO nanostructure from nanoplate to nanowall complex

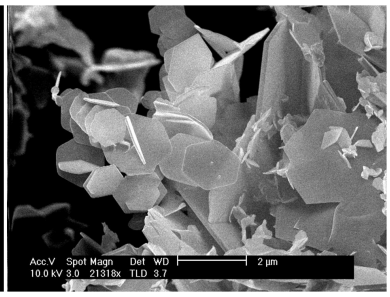
이효반, *유영동, *김봉수

*KAIST 화학과 *KAIST 화학과*

We demonstrate how O2 flow rate affect the formation of NiO nanostructures. The NiO nanostructure has excellent electrochemical property and high performance lithium ion battery. Its electrochemical property depends on 3-dim structures. Although various NiO nanostructures are reported (such as particle, rod, plate, and wall), but how to control of its formation have not been published yet. Here, we show the technique to synthesize the NiO nanostructures from nanoplate to nanowall complex by controlling O2 flow rate. With high O2 flow rate, laterally grown triangular NiO nanoplates were observed. When we reduced flow rate a little, 3-dim NiO plate complex and NiO nanowall complex are existed. The SEM, XRD and TEM help analysis of morphology and crystallinity.







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Synthesis of Phase-Change Nanowires and Study of Their Electrically Driven Memory-Switching Behavior

박이슬, *이진석

*숙명여대 화학과 *숙명여대 자연과학부/화학과*

Chalcogenides exhibit a reversible crystalline-amorphous (order-disorder) phase change induced by temperature or electric field and have been the subject of numerous research activities. Because the phase change is accompanied by dramatic differences in optical reflectivity and electrical resistivity, these materials can be the basis of data storage media such as CD/DVD and phase change random access memory (PRAM).Despite their widespread use, however, the exact mechanism of their phase changes is still under debate. Moreover, the evolution of the phase-change properties as a function of material size has not been fully explored. To learn more about the phase-change mechanism, we synthesized single-crystalline germanium telluride (GeTe) nanowires and nanohelices (NHs), germanium antimony telluride (Ge2Sb2Te5) NWs, and antimony telluride (Sb2Te3) NWs using chemical vapor deposition (CVD) method and investigated the electrical properties of individual nanostructures resulting from their phase transitions. Investigating at the nanoscale the extremes of these nanostructures will offer a fuller sense of the chemistry and physics behind these materials.

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Synthesis of Continuous Oriented AlPO4-5 Films on Glass Substrates

최성은, *이진석

*숙명여대 화학과 *숙명여대 자연과학부/화학과*

Aluminophosphate AlPO4-5, with an AFI structure, is composed of alternating AlO4 and PO4 tetrahedra, forming a framework with one-dimensional, electrically neutral cylindrical pores of uniform cross section (7.3 Å) that are extended parallel to the long (c) axis of the crystal. Controlling the orientation of the subnanometer-sized channels of AlPO4-5 and related molecular sieves is of particular interest for size-selective chemical sensors, separation membranes, and optical systems and has been the subject of many investigations.Here, we present a novel growth technique for synthesis of oriented AlPO4-5 molecular sieve films on glass substrate without seed. As controlling synthetic gel composition, we were able to produce non-intergrown or highly intergrown AlPO4-5 films that exhibit very good orientation on glass substrates.

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Silver Nanowires Synthesis via Different Injection Rates of AgNO3 and Poly(Vinyl Pyrrolidone)

김선화, *이진석

*숙명여대 화학과 *숙명여대 자연과학부/화학과*

Silver nanowires with well-defined dimensions represent a particular class of interesting nanostructures to synthesize and study because bulk silver exhibits the highest electrical and thermal conductivity among all metals. Silver is also an important material that has been used in a rich variety of commercial applications, and the performance of silver in these applications could be potentially enhanced by processing silver into 1D nanostructures with controllable dimensions and aspect ratios. Although a number of approaches, the most widely used method for generating metallic nanowires is still template-directed synthesis that involves either chemical or electrochemical depositions. Here, we concentrate on a soft solution-phase approach for the production of silver nanowire with uniform diameters and in large quantities. The first step of this synthesis involved the formation of Ag seeds by reducing AgNO3 with ethylene glycol at 180 °C. Subsequently, solutions of AgNO3 and poly(vinyl pyrrolidone) in ethylene glycol were added dropwise with different injection rates to this hot solution that contained metal seeds. Silver nanowires could nucleate and grow on these preformed seeds, with various morphology and yields as injection rates.

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Synthesis and characterization of ternary and quaternary silicide nanowires

김현주, *인준호, *김봉수

*KAIST 화학과 *KAIST 화학과*

We report the facile synthesis of ternary and quaternary silicide nanowires showing superconducting or ferromagnetic properties. In this work, metal foils are employed as a substrate and a precursor to achieve multi-component silicide nanowires. Furthermore, we can easily change kinds of metal foil, powder and metal halide. We are investigating physical properties of as-formed ternary and quaternary silicide nanowires.

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A New Platform for Phospholipase A2 Activity Assay by Using Mass Spectrometry

이지언, 김영관, 민달희

KAIST 화학과

Lipase is an important class of enzymes which is involved in various biological processes ranging from cell signaling process to metabolism of dietary triglycerides. Among them, phospholipase A2 (PLA2) is an enzyme that hydrolyzes fatty acid from phospholipid with the concomitant production of lysophospholipid. PLA2 has an important role in a number of diverse cellular responses, including phospholipid digestion and metabolism, host defense and signal transduction. Currently, several assay methods of PLA2 activity are available that are based on conductance, fluorescence, chemiluminescence, and radio-labeled lipid substrate. These conventional methods necessitate multiple steps and/or extra reagents, which hamper routine applications especially in high-throughput assay. Herein, we describe a new PLA2 assay method based on carbon materials and laser desorption/ionization (LDI) time-of-flight mass spectrometry (MS). This MS based PLA2 assay allowed semi-quantitative analysis of both reactant and product in a single measurement without requiring any label, purification process or additional reagents. Inhibition kinetics was carried out with previously known inhibitors and IC50 values were conveniently obtained by the present assay strategy. We believe that this new LDI-MS based lipase assay platform will be a widely applicable tool in lipase related basic research and drug development.

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Cytotoxicity and Genotoxicity of surface modified Super Paramagnetic Iron Oxide Nanoparticles

홍성철, *이재욱, 이재범

*부산대 나노메디컬공학과 *부산대 나노융합기술학과*

Superparamagnetic iron oxide nanoparticles (SPIONs) have various possibilities of application in biomedicine. They can be used such as improving site-specific drug delivery, magnetic resonance imaging (MRI) contrast enhancement, hyperthermia treatments and so on. SPIONs (Fe3O4) were synthesized by Massart's method. For conjugation with materials, they were either functionalized by 3-aminopropyltrimethoxysilane (APTMS) and trisodium citrate or coated with thin layer of silica by tetraethoxysilane (TEOS). Encapsulated SPIONs can be combined with other materials and help their biological role. We made five kinds of differently surface-modified SPIONs and investigated their biocompatibility in vitro. The cytotoxicity and genotoxicity of SPIONs prepared with functional groups to fibroblastic cells were measured by MTT and Comet assays, respectively. It was found that SPIONs affected the cell viability and DNA stability of L-929 fibroblastic cells in a dose-dependent manner.

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Synthesis of polymer coated CdTe nanoparticles using amphiphilic surfactants and methylmethacrylate

이재욱, Sun Fangfang, *홍성철, *이재범

*부산대 나노융합기술학과 *부산대 나노메디컬공학과*

Extensive studies on nanoscale composites of polymers and inorganic materials have been carried out for the design of fundamental comprehension of physicochemical phenomena in the nanoscale regime and for practical applications in optical and electronic devices and biomedical applications. In this study, we have successfully synthesized polymer coated CdTe nanoparticles using octadecyl-p-vinylbenzyl-dimethylammonium chloride (amphiphilic surfactant) and methylmethacrylate. Through the surface exchanging reaction, surface modified CdTe nanoparticles with octadecyl-p-vinylbenzyl-dimethylammonium are prepared. Subsequently, surface modified CdTe nanoparticle and methylmethacrylate are polymerized by radical polymerization. Synthesized organic-inorganic hybrid materials are characterized by NMR, FT-IR, FL and TEM.

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Physicochemical Characteristics and Biocompatibility of Nanoscale HAp embedded Chitosan Film

Sun Fangfang, *이재범

*부산대 나노융합기술학과 *부산대 나노메디컬공학과*

A nacre-like film was designed and fabricated by a freeze-drying of solid-liquid phase separation and subsequent sublimation assisted compression method. Using this method, highly porous film with sufficient mechanical strength was prepared from chitosan and hydroxyapatite (HAp). The composite film was characterized, e.g., microstructure, mechanical performance, biodegradation and cytocompatibility. The bioactivity of the composite scaffolds was studied by examining the apatite formed on the scaffolds by incubating in simulated body fluid (SBF), and the biodegradability of the film characterized by inductively coupled plasma-optical emission spectrometry (ICP-OES) revealed a significant decrease in both Ca and P concentrations of the SBF after the composite film immersed in the SBF for more than 2 months, which suggests that a bone-like apatite layer might be formed on the composite film, this is consistent with the SEM images of the film after immersed in the SBF. Moreover, the decrease of Ca and P concentrations of SBF is varying by the immersing time, content of HAp and surface area of the composite film. Cytocompatibility of the composite film was carried out by evaluating the viability of L-929 fibroblastic cells exposed to the diluted extracts of the composite films. All these assessment of the film properties indicated that this prepared nacre-like film shows considerable possibility on the cell viability and possess high biocompatibility. It is proposed that this nacre-like film with porous structure may be promising scaffolding materials for drug delivery system and bone-patch engineering because the porous structure of the film and the formation of bone-like apatite can provide a good environment for attachment and growth of osteoblast and osteogenic cells.

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Increased Oxygen Coverage Pt–M (M= Fe, Co, and Sn) Alloy Cathode for the Enhanced Oxygen Reduction Reaction

양대수, 유종성

고려대 신소재화학과

A simple and efficient approach has been developed for synthesis of carbon-supported Pt–M (M= Fe, Co, and Sn) nanoparticles (NPs) that combines homogeneous deposition (HD) of Pt complex species through a gradual increase of pH realized by *in situ* hydrolysis of urea and subsequent uniform reduction by ethylene glycol (EG) in a polyol process, giving control over the size and dispersion of Pt–M (M= Fe, Co, and Sn) NPs.Three catalysts with a similar Pt:M atomic ratio, Pt–Fe (50:50), Pt–Co (50:50), and Pt–Ni (50:50), were prepared for the investigation of Oxygen ReductionReaction(ORR). The excellent electrocatalysis ability of the Pt–M (M= Fe, Co, and Sn) catalysts produced by HD-EG is demonstrated through the etermination of electrochemical surface area and fuel-cell polarization performance.A high metal loading catalyst such as Pt–M (60 wt %)/VC fabricated by the HD-EG method outperforms ones with mid-to-low metal loadings (i.e., 40 and 20 wt %), even at a very low catalyst loading of 0.2 mg of Pt–M $^{cm-2}$ at the cathode, which is for the first time reported for the VC-supported Pt catalysts.

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Darkfield based label-free assays of Amyloid-beta growth on SLB

박안나

서울대 화학부

A century of research has passed since the discovery and definition of Alzheimer disease(AD), the primary common dementing worldwide. However, AD has been considered as a fatal disease due to the absence of diagnosis techniques on early stages as well as effective cure currently. To develope the treatments and advanced diagnosis methods, it is essential to understand the etiopathogenesis of amyloid beta-induced neurotoxicity of AD, especially in terms of the deposition of amyloid beta protein in fibrillar form on neuronal cells. Much effort has been directed towards establishing quatitative in vitro assays of this biological process, however, traditional experimental methods using Congo-red and Thioflavin T exhibit the problems. In this research, I suggest label-free technologies focussed on acheiving the observation of Amyloid beta growth without the requirment for fluorophore marker molecules. ;in particular gold nanoparticles and darkfield microscopy provide advantageous alternatives to traditional methods. Moreover, introducing model membranes for the study of Amyloid beta confers analygous environments with in vivo as lipid membranes have a siginificant role in the amylid beta aggregation process.

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Facile preparation of large pore mesoporous silica spheres and hollow mesoporous silica shells

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 proteins into mesopores, and for the retention of pore space after grafting of organic functional groups. Here, we report a simple strategy for pore expansion of highly monodispersed mesoporous silica spheres based on a novel swelling agent incorporation. Contrary to other methods such as surfactant exchange and swelling agent incorporation, pore expansion and template extraction were achieved in one step using a swelling agent. This simple approach yielded mesoporous silica spheres with pores of about 10 nm. The pore expanded-monodisperse mesoporous silica spheres hold great potentials for applications in biosensors and drug delivery system.

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Salt-Induced Colorimetric Nanoparticle Aggregation Assay for Simple and Rapid Antibody Structure and Activity Evaluation

우정림

서울대 화학부

Evaluating structure and activity of antibodies of interest in a simple and rapid manner would be quite useful. Herein, we introduce a gold nanoparticle probe-based antibody structure and activity test method without using complicated and expensive instruments. In this assay, the conformational change of surface-modified antibodies affects the stability of gold-nanoparticles and results in salt-induced aggregation. Under the same condition, only denatured antibody-modified gold nanoparticle probe was aggregated with existence of 0.2 M NaCl. The degree of nanoparticle aggregation was measured and quantified via color change of the gold nanoparticle probe solution. Also, circular dichroism spectra were compared with our colorimetric results and it is shown that our colorimetric method is more sensitive than conventional circular dichroism spectroscopy, which is a typical method to measure secondary structure of proteins. Moreover, we conducted indirect enzyme-linked immunosorbent assay (ELISA) to detect 3-dimensional activity of antibodies. The results were matched with our colorimetric ones, indicating that this strategy could be applicable to all kind of antibodies and an easy, rapid and cheap method for detecting the conformational change of proteins.

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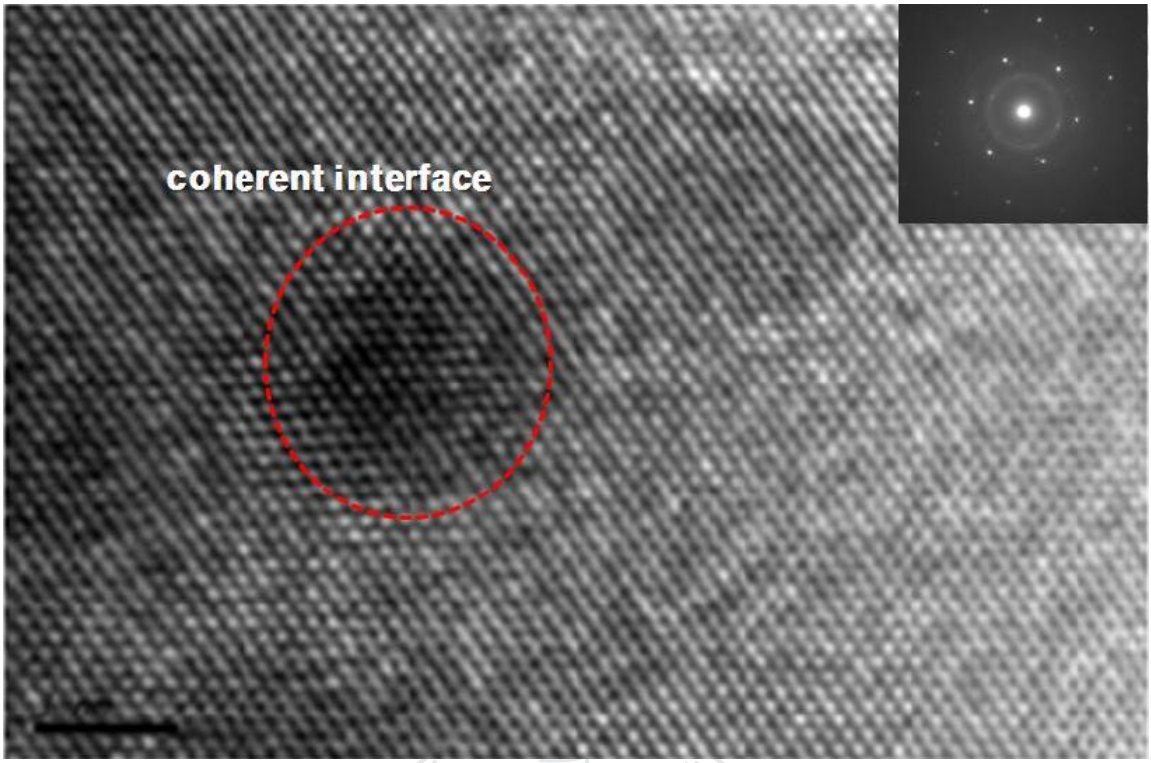
Characterization and microstructures of In2Te3 prepared by insertion of Bi2Se3 nanoparticles

김희진, 한미경, *김성진

*이화여대 화학나노과학부 *이화여대 화학과*

The thermoelectric device ability is measured by figure of merit (ZT). ZT is given by ZT=S2σT /κ (where σ is the electrical conductivity, S the thermo power, and κ 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 In2Te3 prepared by insertion of Bi2Te3 nanoparticles. Bi2Te3 nanoparticles were prepared by solvothermal synthesis.The thermal conductivity and the electrical conductivity decrease with increasing Bi2Te3 nanoparticles contents. The phonons and electrons would be scattered by Bi2Te3 nanoparticles depending on their contents, size. The contents and sizes of Bi2Te3 nanoparticles are critical factor for achieving an increase in ZT compare to In2Te3 bulk. An increase in ZT could be achieved for an optimal contents and sizes of Bi2Te3 nanoparticles.Seebeck coefficient and electrical conductivity have been measured by ZEM-3(Ulvac) and the thermoelectric figure merit calculated.The microstructure and morphologies of In2Te3 insertion of the Bi2Te3 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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Fabrication of Nano-Graphite Hollow Spheres and Their Photoluminescence

박지은, *김성진

*이화여대 화학.나노과학과 *이화여대 화학과*

Water-dispersible graphite multilayered hollow spheres has been developed. Using a soft chemical route of hydrothermal glucose carbonization on double shell Fe3O4@SiO2 templates. The controllability of its nano size and hollow structure, intrinsic optical properties, water solubility, and cell penetration property mean this material might be suitable for biological and medical applications. The resulting nanocomposites were investigated with transmission electron microscopy, X-ray diffraction, ^{29}Si and ^{13}C MAS NMR, Raman, ultraviolet-visible/near-infrared and confocal spectroscopy.

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Metal Nanoparticles Decorated Tin Dioxide Nanowires for Gas Sensing application

김솔, 김성진

이화여대 화학과

Controlled thermal evaporation growth (TEG) allows the achievement of wide band-gap rutile metal oxide(SnO_2) semiconductor nanowires with uniform composition and structural perfection. The growth morphologies are investigated via TEM and XRD analysis. The surface of single-crystalline SnO2 nanowires were further modified with various metal nanoparticles through self-assemblies with polymers. Poly(vinylpyrrolidone) as a stabilizer plays a key role in loading metal nanoparticles onto the surfaces of SnO_2 nanowires. Sensing performance relative to the oxygen-defect metal oxide(SnO_2) rutile nanostructures are also discussed.

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Structure of Bismuth-Telluride Superlattice Nanowire Arrays Fabricated by Electrodeposition in Porous Anodic Alumina Templates

김하영, 김성진

이화여대 화학과

We synthesized bismuth-telluride superlattice nanowire structure in the present of each $Bi(NO_3)_3 \cdot 5H_2O$ and TeO_2 in 1.0 M HNO_3 using porous anodic alumina template. Bi-Te nanowires were deposited electrochemically in regular sequence by pulsed-potential deposition method at room temperature. The pulse potentials for nanowires were selected more negative potential than reduction potential observed from cyclic voltammograms (CVs) and a delay potential was used in no current region between reduction and oxidation potentials of the compound. To obtain dense, highly oriented and single-crystalline superlattice nanowires, the control of the growth rate is critical factor. The microstructure and morphologies of nanowires were investigated by Powder X-ray diffraction and FE-SEM, HR-TEM. Thermoelectric properties (ZT values) of superlattice nanowires are under investigation.

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Drug delivery using biocompatible gold nanoparticles for cancer therapy

유수윤, 장홍제, 민달희

KAIST 화학과

Doxorubicin (DXR) is a frequently used chemotherapy drug in treating a wide range of cancers, including many types of carcinoma, and soft tissue sarcomas. It holds promise as a high potency drug in the fight against cancer and has been in use for decades. In spite of its powerful anti-tumor effects, some of fatal side effects (e.g. cardiomyopathy) and an ever-present risk of extravasation during drug administration can be arisen with the chemotherapy. To overcome those problems, drug delivery system which can reduce toxic side effects and increase efficacy of the therapy can be a very useful apparatus.We synthesized robust and biocompatible gold nanoparticles (AuNPs) using dextran as a reducing agent and surface coating material. Those gold nanoparticles showed the enhanced colloidal stability and dispersion even under harsh conditions like extreme pH, high temperature and salt concentrations. In this report, we prepared DXR-loaded gold nanoparticles as a drug delivery system to more effectively direct DXR to the specific lesion site and reduce its systemic side-effects. We believe that our DXR-loaded nanoparticle could be a candidate system for a tumor-targeted drug delivery in the future.

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Comparative Analyses of Peroxidase Mimic Activity in Different ∝-Fe2O3 Nanoparticles

kiran chaudhari, Nitin Chaudhari, *김민식, *김정호, 김민우, 임신묵, 송민영, **양대수, *유종성

*고려대 소재화학과 *고려대 신소재화학과 **고려대 신소재화학*

Recent serendipitous findings showed that the iron oxide nanoparticles posses intrinsic peroxidase like activity. This particular activity is mostly a surfaced governed phenomenon, with smaller spherical nanostructures showing better activity than their larger counterparts. When similar activity was studied in one dimensional rods, it was interestingly reported that rods with bigger size performed even better than the spherical nanoparticles. This led us to investigate the impact of various physical parameters such as shape; size, surface area, and dimensionality on the peroxidase mimic activity using various ∝-Fe2O3 nanoparticles such as hexagonal prisms-like, cube-like, and rods. It was seen that in multidimensional nanoparticles peroxidase mimic activity is mostly a surface phenomenon, while in rods, it was its one dimensional nature that was responsible in imparting peroxidase mimic activity to rods. Our study of peroxidase mimic activity using different ∝-Fe2O3 will help in better understanding of importance of physical parameters, while developing nanomaterials as artificial enzyme mimetics.

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A Gold Nanoparticle based Strategy for Assay of SARS Corona Virus Helicase Activity

김미희, 장홍제, 유수윤, 민달희

KAIST 화학과

Many diseases caused by virus emerge unexpectedly and threaten our lives continuously. In specific, severe acute respiratory syndrome (SARS) caused by SARS-corona virus (SCV) is a serious type of pneumonia that killed hundreds of people worldwide when it broke out in 2003. Helicase, an enzyme that unwind double stranded nucleic acids into single stranded ones, is essential for viral replication and proliferation. Therefore, helicases have been studied as targets for anti-viral therapy. In this report, we describe a strategy for facile SCV helicase activity assay based on gold nanoparticles. The method allowed quantitative measurement of helicase activity by various analytical principles including UV-Vis absorbance, fluorescence and dynamic light scattering. In contrast to the conventional methods that use radioisotope-labeled nucleic acid or FRET, gold nanoparticle-based system for helicase activity assay possesses advantages such as low-cost, low-volume, rapid readout and compatibility with high throughput assay. We believe that the present strategy will contribute to the growth of clinical diagnostics, mutation detection, and development of anti-virus therapy.

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Carbon-based Materials for Laser Desorption Ionization Mass Spectrometry

곽설진, 김영관, 나희경, 민달희

KAIST 화학과

Matrix-assisted laser desorption/ionization time of flight mass spectrometry (MALDI-ToF MS) rapidly became a powerful tool for biochemical analysis. Although MALDI-ToF MS is well-known for the capability of generating intact macromolecular ions, the presence of interference from organic matrix in the low-mass region makes it less applicable to the analysis of small molecules. To circumvent this problem, matrix-free laser desorption/ionization time of flight mass spectrometry (LDI-ToF MS) has emerged as an alternative approach. The key feature of LDI-ToF MS is the sufficient and controllable transfer of laser energy to vaporize/ionize samples without inducing extensive molecular fragmentation. In this report, we investigated utilities of carbon-based materials—graphene oxide (GO) and multi-walled carbon nanotube (MWNT), specifically—for LDI-ToF MS. Carbon-based materials are thought to trap analytes on their surface and efficiently transfer energy to the analyte. Moreover, carbon-based materials are shown to produce less background ions than other organic matrices and seem to require less laser power for desorption and ionization of analytes. We believe that carbon-based materials have an immense potential for LDI-ToF MS because of those advantageous features.

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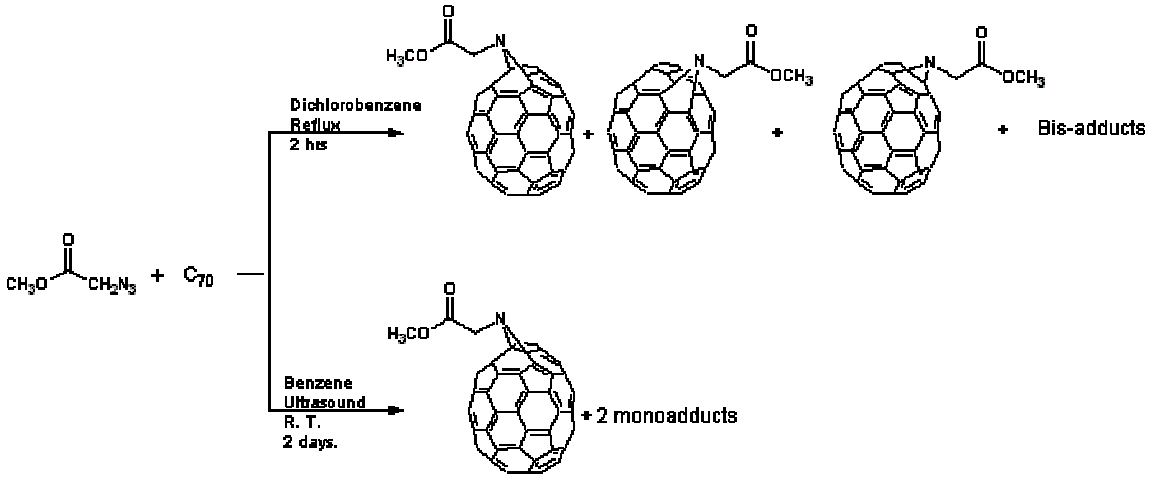
Synthesis of Closed [5,6]-bridged Aziridino[70]Fullerene Derivative under Ultrasonic Irradiation and Self-assembled Multilayer Films

윤신숙, *홍성규, *고원배

*강남대 교양학부 *삼육대 화학과*

Thermal reaction of [70]fullerene with methyl azidoacetate in o-dichlorobenzene produced a mixture of two inseparable regioisomers of the open [5,6]-bridged azafulleroids, the closed [6,6]-bridged aziridinofullerene and the bisadducts in yields of 8.2, 6.8, and 10.3%, respectively. However, under ultrasonic irradiation, the cycloaddition of methyl azidoacetate to [70]fullerene in benzene afforded the closed [5,6]-bridged aziridino[70]fullerene derivative, which was unusual product of cycloaddition to the 5,6-junction of fullerene in 9.1% yield without bisadduct. Its structure was determined by FAB-MS, UV-vis, ^{1}H- and ^{13}C-NMR spectral data. The closed [5,6]-bridged aziridino[70]fullerene-functionalized gold nanoparticle films were self-assembled using the layer-by-layer method on the reactive of glass slides functionalized with 3-mercaptopropyl-trimethoxysilane. The functionalized glass slides were alternately soaked in the solution containing closed the [5,6]-bridged aziridino[70]fullerene and 4-aminothiophenoxide/hexanethiolate-protected gold nanoparticles. The closed [5,6]-bridged aziridino[70]fullerene-functionalized gold nanoparticle films have grown up to 5 layers depending on the immersion time. The self-assembled nanoparticle multilayer films were characterized using UV-vis spectroscopy showed that the surface plasmon band of gold at 527 nm gradually became more evident as successive layers were added to the films



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PEDOT derivative-PANI Electrochromic Device with High Coloration Efficiency and Fast Response

강주희, 최진호

이화여대 화학.나노과학과

A new dual-polymer electrochromic device (ECD) composed of poly(3,4-ethylenedioxythiophene) derivative (PEDOTD) and polyaniline (PANI) electrodes was developed successfully in order to realize synergetic effects in electrochromic (EC) properties such as coloration efficiency (CE) and color-switching rate. From the CE value calculation, we found that the CE of 930 cm2 C-1 for the PEDOTD-PANI ECD is found to be superior to that of other PEDOT-based ECDs reported previously. Furthermore, the present ECDs showed an extremely fast response time of less than 80 ms.

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Inorganic Drug Delivery System for Poorly Water-soluble Drug and Its Bioequivalence Study

오연지, 최진호

이화여대 화학.나노과학과

In this study, we have attempted to encapsulate drug molecules in the montmorillonite (MMT) clay to form organic-inorganic hybrids, where the MMT was considered as a drug delivery carrier. Based on the intrinsic property of clay, we developed a simple way of masking bitter taste and enhancing release efficiency of poorly water-soluble drug (an antipsychotic as a model drug), by intercalation reaction and by subsequent coating with water-soluble polymer like polyvinylacetal diethylaminoacetate (AEA). The content of the model drug in the drug-MMT hybrid was around 25-26 % and that in the AEA treated hybrid was significantly reduced down to 15-16 %. In vitro dissolution test at neutral pH showed that the drug release from the AEA coated drug-MMT was greatly suppressed (< 1%) for the first 5 min, suggesting that the AEA coated drug-MMT be a potential formulation for taste masking of the drug. Notably, in a simulated gastric juice (pH 1.2), the total percentile release of the drug for the first 2 h increased up to 95% for the AEA coated drug-MMT, the profile of which was similar to that of the reference drug, a medication already available on the market. In vivo experiments using Sprague-Dawley rats were also performed to examine the bioequivalence of AEA coated drug-MMT and the reference drug, where the AEA coated drug-MMT exhibited about 20% higher systemic exposure of the drug and its metabolite, as compared with the reference drug. It is, therefore, concluded that a new MMT-based nanovehicle coated with a cationic polymer could be a promising delivery system for both taste masking and solubility enhancement of drugs.

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Inhibition Effect of Alanine and Methionine on the Corrosion of Aluminum in Artificial Sea Water

김현철, 천정균, 김연규

한국외국어대 화학과

Inhibition effects of alanine and methionine on the corrosion of aluminum were investigated in artificial sea water. Based on the low coverage of alanine and methionine we suggested that alanine and methionine adsorption process in aluminum surface is Langmuir isotherm and the carboxyl ion of amino acids seems to be adsorbed on Al.

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Electrooxidation of Glucose at Nanoporous Gold Surfaces : Structure Dependant Electrocatalysis and Its Application to Amperometric Detection

서보라, 김종원

충북대 화학과

Electrocatalytic oxidation of glucose was investigated at nanoporous gold structures electrodeposited on gold surfaces. The nanoporous gold surface (NPG) prepared by electrodeposition of Ag-Au alloy followed by the selective dissolution of Ag is investigated. The morphology and electrochemical surface area of NPG electrodes can be turned by controlling the deposition charges during the formation of Ag-Au layers. As the deposition charge increases, ligament and pore structures become smaller, and surface areas increase. Electrocatalytic oxidation of glucose at -0.1 V becomes more effective at higher deposition charges. Voltammetric responses of NPG surfaces in pure electrolyte solutions and toward ascorbic acid suggest that the electrocatalytic oxidation of glucose arises from the enrichment of (110) or (100) surface orientation of nanoporous gold surfaces as the deposition charge increases. The electrooxidation of glucose at NPG surfaces with higher deposition charges is retained in the presence of Cl^-, which suggests possible applications to the amperometric detection of glucose in biological samples.
[This research was financially supported by the Ministry of Education, Science Technology (MEST) through the Human Resource Training Project for Regional Innovation.]

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Electrocatalysis at Gold Films Electrodeposited from Sulfite-Based Commercial electrolytes

현명희, 김종원

충북대 화학과

A simple one-step electrodeposition method was used to fabricate gold nanostructures on gold electrodes from sulfite-based commercial electrolytes. The morphologies of gold nanostructures can be easily controlled by the variation in electrodeposition charge or electrodeposition potential. As the deposition charge increases, the surface area increases and the surface exhibits higher catalytic performance for the reduction of oxygen. Electrocatalytic oxidation of glucose at 0 V is more effective at higher deposition charges. Voltammetric responses of surface nanostructures suggest that the electrocatalytic oxidation of glucose arises from the enrichment of (110) surface orientation of gold surfaces as the deposition charge increases. The electrooxidation of glucose is retained at surface nanostrucrures in the presence of Cl^-. A sensitive enzyme-free sensor can be easily developed for the detection of glucose. [This research was financially supported by the Ministry of Education, Science Technology (MEST) through the Human Resource Training Project for Regional Innovation.]

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Mo/Glass 표면에서의 CIGS 합성

이상민, 이치우

고려대 신소재화학과

최근의 태양광 시장은 기존의 실리콘 타입 태양전지 못지않게 박막형 태양전지로 변화하는 양상을 보여주고 있다. 그 중에서도 CIGS 박막 태양전지는 광 흡수도가 크고 밴드갭이 적합하여 많은 관심을 받고 있다. CIGS 박막태양전지 제조방법은 크게 세가지, 즉 Target 을 이용한 진공 증착, 전기화학적 (전착) 그리고 코팅 방법들로 나눌 수 있으며, 그 중에 전착을 이용한 CIGS 박막 태양전지는 저온의 전해질 용액 속에서 광 흡수층을 제조하기 때문에 증착보다 제조단가가 낮고 높은 효율, Role to Role 공정에 따른 대면적 모듈 생산이 가능하므로 대량 생산 가능성이 높다.본 연구에서는 저비용 고효율의 전착 방법을 이용하여 CIGS 박막을 제조하였다. 전기화학법을 이용하여 전해질 수용액 내에서 Cu2+, In3+, Ga3+, Se4+ 성분 이온들이 환원되는 전압을 걸어 주어 CIGS 박막을 제조하고 그 조성을 분석하였다. Mo/Glass 표면 위에 CIGS 층을 전착 시키고, SEM 을 사용하여 전착된 표면의 모폴로지를 분석하였으며, EDS 로 전착물의 조성을 측정 분석하였고 XRD 를 이용하여 그 구조를 조사하였다.

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ZnO Nanopillar Arrays on Si Substrates Prepared by Electrochemical Deposition

최익호, 이상민, 이치우

고려대 신소재화학과

ZnO 는 넓은 밴드갭(3.37eV)과 높은 엑시톤 결합에너지(60meV)를 가지고 있어 다양한 분야에서의 응용 가능성이 확인되고 있다. n 형 / p 형 ZnO 접합 나노 다이오드 성장, 전이 금속 도핑을 통한 전하 운반 농도의 자유로운 제어 등과 관련된 새로운 합성 기술, 원하는 위치에서 단일 ZnO 나노와이어를 성장시키는 기술 등 많은 응용 가능성이 있다.본 연구에서는 상온 1 기압에서 삼전극 (working electrode = Si , counter electrode = Pt , reference electrode = Ag/AgCl)을 이용하는 전기화학적 전착법으로, 전해질의 농도와 반응 온도, 전착 전압, 전착시간에 변화를 주어 ZnO 나노필러 어레이를 합성 한 후 SEM 을 이용하여 표면을 관찰하는 연구를 수행 하였다. ZnO 전착에 가장 효율적인 환경을 확인 후 생성 시료에 대해 UV, PL, XRD 분석을 하였다.

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전극표면의 금속 UPD layer의 대체에 의한 금속 단원자층 침적

윤상효, *Deyu Qu, 이상민, 이치우

*고려대 신소재화학과 *Korea University*

금 전극에 Cu UPD 단일층을 형성하고 이를 백금으로 대체시킴으로써 백금 층을 형성하고자 하였다. 이 방법을 사용하는 경우에서는 백금의 담지량을 크게 줄일 수 있을 뿐만 아니라 백금의 분산도를 높게 할 수 있기 때문에 DMFC 등에서 촉매로 사용하는 경우에서 높은 전기활성 (electroactivity)과 전력 밀도(power density)를 얻을 수 있을 것으로 예상된다. 본 연구에서 사용한 금속 침적방법에서는 Au(111) single crystal electrode 에 underpotential deposition (UPD) Cu 를 통해 Cu monolayer 를 형성하고, Cu monolayer 에 Pt 가 자발적으로 비가역적 산화환원 반응을 함으로써 Pt monolayer 로 대체된다. 이 과정에서는 Cu 가 산화되고 Pt 가 환원되는 동시에 흡착된다. Pt 흡착은 Au(111)표면 끝부분 전체에 특별한 흡착방법 없이 금속에 균일하게 침착 된다. 일반적인 전착에서 Au(111)표면에 Cu deposition 되는 정도를 다르게 함으로써 Pt 흡착되는 정도를 비교할 수 있다. 제조된 금 나노 입자와 UPD Cu/Au 의 형태 및 원소 조성은 주사전자현미경 (SEM)과 에너지 분산 분광계 (EDS)를 이용하여 분석 할 수 있으며, 금 전극에 흡착된 백금의 전기촉매적 특성은 CV 를 이용하여 측정할 수 있다.

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Large-scale Synthesis of Magnetite Nanocrystals Imbedded in Carbon Matrix and Their Application in Lithium-ion Batteries

박원철

서울대 융합과학기술대학원 나노융합학과

The rechargeable lithium-ion batteries have been widely used as power sources for various portable consumer electronics such as notebooks, digital cameras, and cellular phones during the past decade. Moreover, they have also attracted growing attention as power supplies of electric vehicles and hybrid electric vehicles. The market demand of reduced cost, high specific energy density and good cycling performance is increasingly required. Accordingly, a great deal of effort has been made to find alternative electrode materials with improved electrochemical performance for lithium-ion batteries. The use of nanosized anode materials has been a popular way to get high energy density and long cycle preformance. Among various transition-metal oxide naostructured anode materials, iron oxide nanomaterial exhibit advantages of low cost and environmental benignity, which make it a kind of promising anode material. In the present study, we report on a facile large-scale synthesis of magnetite nanoparticles imbedded in carbon matrix. The structure and morphology of the resulting nanocomposite is investigated with X-ray powder diffraction, raman spectroscopy, scanning electron microscopy and transmission electron microscopy. Cyclic voltammetry and cyclic test of the nanocomposite as anode material for lithium ion batteries were also studied. The magnetite-C nanostructured material shows a very high specific capacity in the initial cycle and high capacity retention, exhibiting potential application as anode material in lithium-ion batteries. The superior electrochemical characteristics benefit from the uniform distribution of magnetite nanoparticles, proper nanostructure, good conductivity as well as the prevention of the aggregations by carbon nanoshell during the cycling.

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용액을 사용한 Silicon Nanowire 제조

금상준, 이상민, *이치우

*고려대 신소재화학 *고려대 신소재화학과*

실리콘 나노와이어는 우수한 전기적, 광학적, 기계적, 열적 특성을 가지고 있기 때문에 큰 관심을 받아왔다. 실리콘 나노와이어는 초소형화된 고집적회로, 고효율이 실현되는 최첨단 이점을 가진 미래산업의 주요 소재로 사용 가능하다. 본 연구에서는 상온 1 기압에서 실리콘의 액상 식각 방법을 통하여 Silicon nanowire 를 제조하였다. 실험에 사용된 실리콘은 P-type, B-doped Silicon(100) (4-7Ω ㎝)의 wafer 이었으며, HF 용액의 농도와 반응시간 변화를 통하여 실험을 진행하였다. 실험조건 변화에 따른 와이어의 생성 속도와 직경, 두께 변화의 특성에 대하여 조사하였다. 실험을 통하여 얻어진 실리콘 와이어의 크기 등 물성변화는 Scanning electron microscopy (SEM), JEOL 5600 microscope 를 이용하여 확인하였다.

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Platform for highly sensitive alkaline phosphatase-based immunosensors using 1-naphthyl phosphate and an avidin-modified indium tin oxide electrode

라지불, 양해식

부산대 화학과

We report a versatile platform for highly sensitive alkaline phosphatase (ALP)-based electrochemical biosensors that uses an avidin-modified indium tin oxide (ITO) electrode as a sensing electrode and 1-naphthyl phosphate (NPP) as an ALP substrate. Almost no electrocatalytic activity of NPP and good electrocatalytic activity of 1-naphthol (ALP product) on the ITO electrodes allow a high signal-to-background ratio. The effective surface covering of avidin on the ITO electrodes allows very low levels of nonspecific binding of proteins to the sensing electrodes. The platform technology is used to detect mouse IgG with a detection limit of 1.0 pg/mL.

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Ultrasensitive Detection of DNA in Diluted Serum Using NaBH4 Electrooxidation Mediated by $[Ru(NH_3)_6]^{3+}$ at Indium–Tin Oxide Electrodes

이정아, 양해식

부산대 화학과

There is a crucial need for simple and highly sensitive techniques to detect DNA in complicated biological samples such as serum. Here we present an ultrasensitive electrochemical DNA sensor using (i) single DNA hybridization with peptide nucleic acid (PNA), (ii) selective binding of [Ru(NH3)6]3+ to hybridized DNA, (iii) fast NaBH4 electrooxidation mediated by [Ru(NH3)6]3+, and (iv) low background currents of NaBH4 at indium–tin oxide (ITO) electrodes. The [RuIII(NH3)5NH2]2+ formed from [RuIII(NH3)6]3+ in borate buffer (pH 11.0) is readily electrooxidized to both [RuIV(NH3)5NH2]3+ and Ru complex with a higher oxidation state. In the absence of [Ru(NH3)6]3+ bound to the DNA-sensing ITO electrodes, the oxidation currents of NaBH4 are very low. However, in the presence of [Ru(NH3)6]3+, the oxidation currents of NaBH4 are highly enhanced due to electron mediation of the oxidized Ru complexes. PNA and ethylenediamine on DNA-sensing electrodes significantly decrease [Ru(NH3)6]3+ binding, also allowing for high signal-to-background ratios. All combined effects enable the detection of DNA with a detection limit of 1 fM in 10-times diluted human serum.

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Fast Catalytic and Electrocatalytic Oxidation of Sodium Borohydride on Palladium Nanoparticles and Its Application to Ultrasensitive DNA Detection

강현주, 양해식

부산대 화학과

We report an ultrasensitive DNA sensor using the rapid enhancement of electrocatalytic activity of DNA-conjugated Pd nanoparticles (NPs). The DNA detection offers an ultralow detection limit, a wide detection range, and a short incubation time. The rapid enhancement comes from the fast catalytic hydrolysis of NaBH4 and subsequent fast hydrogen sorption of Pd NPs. The highly enhanced electrocatalytic activity of DNA-conjugated Pd NPs allows high currents for NaBH4 electrooxidation within potential windows. The superior sensor performance along with the simple preparation and detection procedure makes our protocol highly viable for practical applications.

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Properties of Ti doped $LiFePO_4$ cathode material for Li ion secondary battery

홍경수, 한현주, 진종성, 정의덕

한국기초과학지원연구원 하이테크부품소재연구지원센터

In order to improve the electrochemical properties of $LiFePO_4$, we synthesized Ti-doped $LiFePO_4$ powders by using the solid state reaction method with different amount of titanium ions. All materials were annealed in the reduced atmosphere with different amount of titanium and characterized. The powders annealed at 650°C showed the best crystallization via XRD analysis. The surface conditions and the states of metal ions were checked by using the SEM and XPS. Bare $LiFePO_4$ shows about 14% decrease of the capacity after 50times of charge-discharge cycles. We observed that the Ti-doping increased the charge-discharge life cycle because $LiFeP_{0.95}Ti_{0.05}O_4$ powder showed less than 5% decrease of the capacity.

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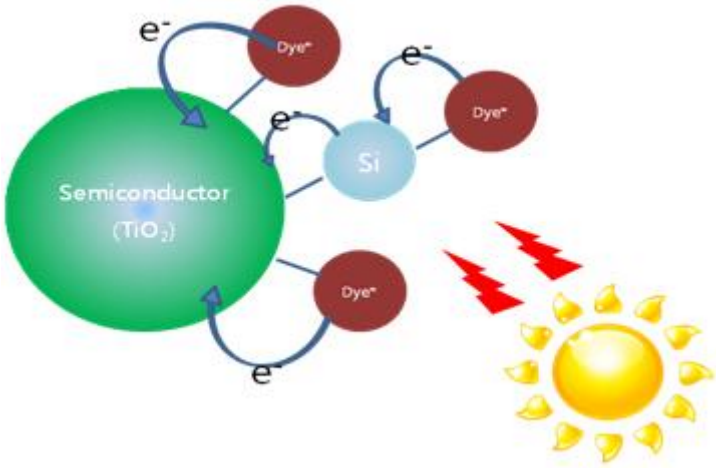
Functionalization of silicon nanoparticles via silanization for application to dye–sensitized solar cells

하은성

고려대 화학과

Highly efficient dye–sensitized solar cells (DSSCs) through enhancing the short–circuit photocurrent density by incorporating functionalized Si nanoparticles (Nps) into the TiO_2 film of the DSSCs have been developed. The incorporation of functionalized Si Nps into the 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 carboxyl acid 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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Additive effects in the modification of prussian blue analogue films for flexible electrochromic device

정영희, 곽준영, 김영일

부경대 화학과

Electrochromism is the phenomenon displayed by some materials of reversibly changing color when external potential is applied. The electrochromic device mostly consists of several layers. Prussian blue analogues have anodic electroactive layer, change their optical properties by switching between their oxidized and reduced form. For commercial use, high-contrast ratio and long term stability are very important factor. the cationic surfactant cetyltrimethylammonium bromide(CTAB) is able to modify, control the properties of electrode surfaces and enhance reaction rates. Ruthenium is able to form very stable mixed-valent Ru-oxide inorganic films cross-linked by cyanide. For improving the electrochemical activity and stability, CTAB and RuCl3 were added into PB analogue coating solutions. Modified PB analogue films were prepared by sol-gel coating and electrodeposition onto flexible ITO substrate. Modified PB analogue films were characterized using XRD, SEM, TEM, Cyclic voltammetry and electrospectrophotometer.

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Development of Miniaturized Electrochemical Sensors for Point-of-care and Laboratory Testing

강태영, 김현숙, 김민수, 신정원, *남학현, *차근식

*(주)아이센스 부설연구소 *광운대 화학과*

When we think of applications of miniaturized sensor technology in clinical diagnostics we specifically have in mind point-of-care (POC) settings. In the past, the cost and/or analytical performance of these technologies have limited the application of the new sensor technology in traditional laboratory settings. However, recent improvements in technology and manufacturing methods have allowed the fabrication of miniaturized sensors and analyzers that combine the ease-of-use and portability required in POC with the accuracy, reliability and cost-effectiveness of traditional systems. The i-Smart 30 electrolyte analyzer is a definite example of such a system. The i-Smart 30 analyzer, developed by i-SENS, is a fully automated electrolyte analyzer that can accurately measure the concentrations of sodium, potassium, and chloride ions and hematocrit in blood for POC and laboratory testing. The analyzer uses 60 μl of whole blood, serum, or plasma for analysis and reports the results in fifty seconds from sample introduction on the color screen of the analyzer. Besides many advantageous features mentioned above, the i-Smart analyzer is the only electrolyte analyzer available in the market that uses a closed cartridge including electrochemical sensors, calibration solutions, and all fluidic components from a sample introducing probe to a waste bag. This cartridge reduces the maintenances of the analyzer and relating labor, time, and expense. The electrochemical sensors in the i-Smart cartridge are all formed by screen-printed electrodes on a PET (polyethylene terephthalate) substrate with approximate dimensions of 38x27 mm. The sensors for electrolytes are all based on the principle of ion-selective electrodes (ISE). That is, an electrical potential can be established across a membrane that is selective to a specific ion. The ISE, with the exception of hematocrit and reference electrodes, are formed from layers of polymer membranes that are bonded to the substrate. The reference electrode is an open liquid junction between Ag/AgCl electrode and sensor chamber. Hematocrit is determined by measuring conductivity of the sample. The measurement is based on the principle that the resistivity of blood increases as the concentration of cells

increases due to high resistance of the cell membrane. The sensor chamber contains two electrodes for measuring conductivity. The performance of ISE and hematocrit electrodes were evaluated with the i-Smart 30 analyzers. Whole blood samples were analyzed on the i-Smart 30 analyzers and an ABL 825 blood gas analyzer (Radiometer) for comparison. For hematocrit, the results were also compared to the centrifuged microhematocrit method. In conclusion, the i-Smart 30 electrolyte analyzer shows good correlation in whole blood with the ABL 825 blood analyzer for sodium, potassium, chloride, and hematocrit. The excellent analytical performance of the i-Smart 30 electrolyte analyzer clearly demonstrates the utility of miniaturized electrochemical sensors in clinical diagnostics.

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Synthesis of Functionalized Si Nanoparticles and their Application to Dye-Sensitized Solar Cells for Enhanced Performance

이승주

고려대 화학과

The highest energy conversion efficiency of dye-sensitized solar cell (DSSCs) has been achieved with ruthenium-bipyridine dyes (Ru(II) dyes). But the efficiency of the DSSCs using Ru dyes has been remained at approximately 11% for the last several years. To improve the performance of DSSCs, we try to search for the ideal type of dyes which is to sensitize Tio_2 over the entire visible spectral range and to possess their high molar absorption coefficients. We present here the improved performance of the DSSC with Tio_2 film modified with functionalized Si nanoparticles(nSi). The incorporation of the functionalized nSi into the Tio_2 film is expected to extend the light absorption spectral region more toward longer wavelengths than that achieved by widely used Ru(II) dyes. Moreover, the nSi functionalized with appropriate groups such as COOH can link between Tio_2 and Dyes. The nSi treated on Tio_2 film are expected to provide more sites for dye adsorption compared to untreated Tio_2 film. We also try to control the size of the nSi to study different aspects arising from the size of the nSi. The nSi were prepared by reducing $SiCl_4$ with $LiAlH_4$ in the presence a surfactant and subsequently functionalized to form nSi-COOH by the reaction with acrylic acid (R. D. Tilley, S. Saito, Langmuir, 19 (2003) 5115). We introduce a new concept using stabilizing agent to control the size of nSi. The functionalized nSi have been characterized by HR-TEM, UV-Vis absorption spectrometry, FT-IR, and ^{1}H-NMR. The influence of incorporation of the functionalized nSi into the Tio_2 film on the performance of the DSSCs has been investigated by using *J-V* curves of DSSCs consisting of Tio_2 film with the nSi-COOH.

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Synthesis of functionalized Ge nanoparticles for enhanced photocurrent of dye-sensitized solar cells

최용선

고려대 화학과

Dyesensitized solar cells (DSSCs) have attracted much attention because of their high photon-toelectricity conversion efficiency. But the efficiency of the DSSC using Ru(Ⅱ)-bipyridine dyes has been remained at approximately 11% for the last several years. Because the Ru(Ⅱ)-bipyridine dyes absorb the limited wavelength region of solar radiation. Ge nanoparticles were used as co-sensitizer for DSSCs aiming at the extension of their absorption to the longer wavelength region than that achieved by widely used Ru(Ⅱ)-bipyridine dyes. The Ge nanoparticles were synthesized in the solution phase at room temperature and functionalized with carboxylic acid group which could be attached to the TiO_2 film (E.Fok, M.Shin, A. Meldrum, J. G. C. Veinot, Chem. Commun. (2004) 386). The Ge nanoparticles were prepared by reducing GeI_4 with $LiAlH_4$ in the presence of a surfactant and subsequently functionalized to form Ge-COOH by the reaction with acrylic acid. The functionalized Ge nanoparticles were characterized by HR-TEM, FT-IR spectroscopy, UV-Vis absorption spectroscopy and ^{1}H-NMR. The influence of incorporation of the functionalized Ge nanoparticles into the TiO_2 film on the performance of the DSSCs was investigated through photocurrent-voltage characterization.

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Sensitivity enhancement of a glucose biosensor adopting conducting polymer nanofiber structures.

정신환, *이영관, 손용근

*성균관대 화학과 *성균관대 화학공학과*

A bundle of nanofiber/tubule structures comprised of conducting polymer was fabricated onto an ITO electrode to enhance current collection efficiency. A glucose biosensor adopting the bundle system was manufactured by capturing enzyme of glucose oxidase covered with a thin Nafion film. Chronoamperometric current response from the oxidation of the hydrogenperoxide was measured. The glucose substrate was allowed to pass through the Nafion membrane from the bulk test solution to the enzyme. The enzyme can produce hydrogenperoxide and its oxidation current was measured with a constant potential. This sensor provided a current response linear dependent on the concentration of the substrate. The manufacturing procedure was stuied with SEM images.

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One-step synthesis of silver nanoparticles and effect of reducing temperature for ink-jet printable silver ink

이승현, *이영관, 손용근

*성균관대 화학과 *성균관대 화학공학과*

Synthesis of ink-jet printable silver nanoparticles by chemical reduction using formaldehyde (HCHO) was studied in this work. Reduction temperature had an effect on size of synthesized silver nanoparticles. Effect of promotive agents such as sodium hydroxide and sodium carbonate and reduction time were investigated. Synthesised ink-jet printable silver nanoparticles were well dispersed into aqueous solution. In order to control printable viscosity of dispersed silver colloid inks, we introduced the co-solvent such as water/diethylene glycol(DEG). Products were characterized by using UV/Vis spectroscopy, high resolution transmission electron microscopy(HRTEM) and atomic absorption spectroscopy(AAS). The silver colloid inks for further electronical applications were stable for long time.

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The molecular- ruler fabrication of Metal-insulator-semiconductor structure for molecular devices

최동철, 손용근

성균관대 화학과

Nano-scale organic dielectric layers for organic thin film transistor (OTFT) were synthesized by the molecular-ruler method. Molecular-ruler method has been known as a good process to fabricate nano-scale structures for nano-devices with the advantages of low cost and high throughput. In this work, 16-mercaptohexadecanoic acid (16-MHDA) was used to make compact layers on gold substrate by self-assembled monolayer (SAM), and Cu2+ from Copper(Ⅱ) perchlorate was also used as a linker ion between 16-mercaptohexadecanoic acid (16-MHDA) layers. Multiple layer-by-layer structures of 16-mercaptohexadecanoic acid (16-MHDA) and Cu2+ were fabricated. Finally Metal-insulator-semiconductor (MIS) structure was manufactured by covering the multiple structure with conducting polymer layer. X-ray fluorescence (XRF) spectroscopy, x-ray photoelectron spectroscopy (XPS), cyclic voltammetry (CV), infrared (IR) spectroscopy and scanning electron microscope (SEM) methods were utilized to verify the character of these structures.

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Electrocatalytic Activity of Metal Nanoparticles/CNT-based Electrocatalysts for Oxygen Reduction Reaction

김연수, *심준호, **이영미, ***이종목

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Metal nanoparticle-carbon nanotube composites (M/CNTs) are attracting growing interest in catalysis for the fuel cell development due to their unique properties such as their large surface area-to-volume ratios, stability, and high electrical conductivity. Here we present the synthesis and electrochemical characterization of various M/CNT-based nanostructured materials (M = Pt, Pd, Ir, Au, Ag, and Ru). M/CNTs were synthesized by modified polyol process at high pH. The electrocatalytic activities of the prepared catalysts were evaluated for the oxygen reduction reaction (ORR) using rotating disk electrode experiments in acidic (0.5 M H_2SO_2) condition. The molecular oxygen reduction at Pd/CNT electrode started at more positive potential than that at any other metal doped CNTs. Our results revealed that Pd/CNTs possess remarkable catalytic activity and high stability for ORR in acid media, which implies the potential application of the Pd/CNTs as a cathode material of 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, ROK.

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Size-controlled Carbon-supported Pd Nanoparticles (Pd NP-C) for Oxygen Reduction Reaction

정현정, *심준호, **이영미, ***이종목

*이화여대 화학나노과학과 *이화여대 신재생에너지연구센터 **이화여대 자연과학대학/화학전공 ***이화여대 화학과*

Recently, extensive research has been performed to develop non- electrocatalysts for the efficient four-electron oxygen reduction reaction (ORR) due to the high cost of Pt, most commonly used cathode catalyst in fuel cells. As one of these research efforts, we synthesized size-controlled carbon-supported Pd nanoparticles (Pd NP-C) in the presence of various concentrations of poly(*N*-vinylpyrrolidone) (PVP). The synthesized Pd NP-C then characterized by XRD, SEM/EDS, TEM, and electrochemical methods. The rotating disk electrode (RDE) experiments at the various Pd NP-C modified glassy carbon electrodes in acidic media confirmed the ORR occurred via single-step four-electron transfer at these electrodes (i.e., nearly complete reduction of O_2 to H_2O). The higher the concentration of PVP, the more positive shift in the onset potential of ORR is also observed.This research was carried out under the General R/D Program of the Daegu Gyeongbuk Institute of Science & Technology (DGIST), funded by MEST, ROK.

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pyridinium iodide 종류의 이온성액체를 이용한 염료감응 태양전지용 전해질

전세미나, *한치환, 김강진

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1991 년 스위스 EPFL 의 Grätzel 그룹에서 광전변환 효율이 높은 액체 전해질을 사용하는 염료감응 태양전지를 발표하였다. 보통 액체 전해질에는 유기 용매, I^{3-}/I^{-} redox couple 과 첨가제가 들어가는데, 이때 첨가제로는 pyridine 유도체와 리튬염이 광전류를 향상시키는 효과가 있다. 이와 같은 효과를 위해 이온성 액체도 넣게 되는데, 이로 인해 전해질 용액의 점도를 높이게 됨으로써 이온들의 확산성이 떨어지게 되고 따라서 광전류도 떨어지게 되는 요인이 된다. 그러므로 점도를 낮추기 위한 많은 이온성 액체들 중 imidazolium cation 의 이온성 액체가 널리 연구되어 왔다. 이번 실험에는 imidazolium cation 의 이온성 액체를 이용한 전해질과의 비교를 통해 좀 더 점도가 낮은 pyridinium cation 의 이온성 액체 중 하나인 1-hexylpyridinium iodide 를 이용한 전해질을 사용하여 short-circuit photocurrent density 는 17.75 mA/cm^2, open-circuit voltage 는 0.696 V, 광전변환 효율은 7.92%인 염료감응 태양전지를 얻을 수 있었다.

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Modification of Ni Cathode Material for Molten Carbonate Fuel Cell

최희선, *이철우, 김건

*고려대 화학과 *성신여대 화학과*

Many investigators have attempted to obtain an alternative molten carbonate fuel cell (MCFC) cathode. In this study, we have synthesized Co/Nb-coated NiO as a new alternative MCFC cathode material. The Co/Nb-coated Ni powders as a new cathode material of MCFC have been successfully prepared using a polymeric precursor based on the Pechini method. Thermal gravimetric analysis (TGA) was performed to investigate the thermal behavior of the gel precursors. X-ray diffraction (XRD) and scanning electron microscopy/energy dispersive spectroscopy (SEM/EDS) were employed in characterization of NiO cathode. The dissolved nickel in the molten carbonate was analyzed quantitatively by inductive coupled plasma-mass spectroscopy (ICP-MS). The cell voltage evolutions of single cells with pure NiO and modified NiO cathodes coated with Co and/or Nb for 300 hours operation at 150 mA/cm2of current density. The electrochemical cell performance with Co/Nb-coated NiO cathode is higher than pure NiO and Co-coated NiO cathode. The solubility of decreasing amount of Nb in Co-coated NiO cathode was less than the pure NiO, Co-coated NiO cathode. Consequently, the Co/Nb-coated NiO cathode can be used as a candidate cathode material for MCFC.

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Synthesis and Characterization of New Porous Sulfonated poly(fluorinated arylene ether)/Poly(N-vinylimidazole) Blend Polymer Membrane for Anhydrous High Temperature PEMFCs

이종원, *이철우, 김건

*고려대 화학과 *성신여대 화학과*

Acid-base polymer complexes represent an effective approach to development of proton conducting membranes. Basic polymers doped with an amphoteric acid acts both as a donor and an acceptor in proton transfers and allows the proton to migrate. Acid-doped poly[2,2'-(m-phenylene)- 5,5'-bibenzimidazole](PBI) and poly(2,5-benzimidazole)(ABPBI) have been studied as a membrane for high temperature PEMFCs. These membranes show high proton conductivity and CO tolerance at high temperature. In the previous study, the H_3PO_4-doped sulfonated poly(fluorinated arylene ether)s (SDF-F)/poly(N-vinylimidazole) (PVI) blend membrane was successfully synthesized, the membrane had good physicochemical, thermal stability. In the present study, we report a concept about the formation of pores in SDF-F/PVI blend polymer electrolyte membrane to increase the ionic conductivity of the membranes. In order to prepare the new polymer electrolyte membrane, nano size spherical SiO_2 composite SDF-F polymer membrane was removed with HF solution. The porosity of the membrane can be controlled with the different amount of SiO_2. The new SDF-F/PVI blend membrane was prepared by soaking the porous SDF-F in PVI aqueous solution. The structural, thermal, chemical, and electrical characterization of new porous membranes doped with H_3PO_4 were investigated by scanning electron microscopy (SEM), energy dispersive spectroscopy (EDS), thermal gravimetric analysis (TGA), Fourier transform infrared spectroscopy (FT-IR), electrochemical impedance spectroscopy (EIS) and single cell test. Acknowledgements : This work was supported by the ERC program of MOST/KOSEF (grant No. R11-2002-102-00000-0) and Seoul Renewable Energy Research Consortium (Seoul R & BD Program).

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Synthesis of nanosized spherical V_2O_5/polythiophene composite powder for lithium batteries

김주성, *여인형, **조원일, ***모선일

*아주대 화학과 *동국대 화학과 **KIST 에너지환경연구부 ***아주대 에너지시스템학부*

Safe, high-energy-density, and long-lasting rechargeable lithium batteries are urgently needed in today's information-rich, mobile, and energy-conscious society. For lithium secondary battery cathodes, nano structured vanadium pentoxide (V_2O_5), has been attractive because of its essential advantages of its structural flexibility with lithium intercalation. In this work, size controlled nanospherical V_2O_5 can be synthesized by a hydrothermal methode from a precursor, $VO(acac)_2$, that was formed by refluxing V_2O_5 in acetylacetone(acac). Composite powders of nanostructured V_2O_5 and conductive polymers are made, in order to increase the conductivity of the electrodes. Polythiophene(PTh) is of great interest in recent years because of the low cost of its monomer, the high redox potential, the chemical stability and high conductivity. The composite powder can be synthesize by adding an oxidation catalyst solution to the thiophene monomer containing the dispersed V_2O_5 nanospheres. The characteristics and its performances were investigated by scanning electron microscopy (SEM), X-ray diffraction (XRD), charge-discharge cycle test and cyclic voltammetry (CV) using multichannel battery test mode.

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Determination of acetaminophen by a Novel Ruthenium(II) Complex Modified Electrode

손정익, *원미숙, 심윤보

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A novel ruthenium(II) complex, [$RuC1_2(DMSO)_2$(PhenTPy)] has been synthesized by the condensation of $RuCl_2(DMSO)_4$ with (1-(1,10-phenanthrolinyl)-2,5-di(2-thienyl)-1H-pyrrole)[PhenTPy] in a $CHCl_3$ solution. Various techniques UV-visible spectroscopy (UV), mass spectroscopy (MS), and cyclic voltammetry (CV) were employed to characterize the [RuC12(DMSO)2(PhenTPy)] complex. Poly-[$RuC1_2(DMSO)_2$(PhenTPy)] complex modified electrode has been fabricated via electropolymerization of [$RuC1_2(DMSO)_2$(PhenTPy)] complex in 0.1 M TBAP/CH_2Cl_2 solution. The modified electrode exhibited an electrocatlytic activity towards the oxidation of acetaminophen in phosphate buffer solution. Using amperometry method, the lowest detection limit of 7.9 x 10^{-6} M (n = 9) was achieved for acetaminophen determination. The poly-[$RuC1_2(DMSO)_2$(PhenTPy)] modified electrode promises to be potentially helpful for a numerous of sensing in environmental and biomedical applications.

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Enhanced electrochemical of surface-modified ZnO electrode by TiO_2 coating

이상헌, *이철우, 김건

*고려대 화학과 *성신여대 화학과*

Rechargeable Ni/Zn batteries represent a very attractive power supply with the advantage of reduced environmental impact compared to the Ni-Cd system and are much less expensive than Ni-MH batteries. The Ni/Zn battery delivers very high specific energy(55-85Wh/kg) and high specific power(140-200W/kg) and the nominal cell voltage of 1.6V is 400mV higher than for Ni/Cd and Ni/MH batteries. The biggest problems in rechargeable Ni/Zn batteries are the Zinc shape change, dendrite formation and high dissolution of the zinc electrode that occur with increasing number of charge/discharge cycles. In this study, we have tried to prepare a new alternative anode material by the TiO_2-coated ZnO powder using polymeric precursor based on a sol-gel method. The surface-modified and pristine ZnO powders were characterized by X-ray diffraction (XRD), transmission electron microscopy (TEM). For the zinc dissolution test, the concentration of Zinc in the electrolyte was measured by inductive coupled plasma-Auger electron spectroscopy (ICP-AES). The Shape change of TiO_2-coated ZnO electrode could be restrained effectively, and the discharge capacity of the cells would keep much more stable than that with the pristine ZnO.

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Effects of MWNT incorporation on DSSC performance : electrochemical impedance spectroscopic studies

황윤화, 표명호

순천대 화학과

Since Grätzel et al. discovered efficient solar energy conversion based on TiO_2 / Ru complexes / redox couple, Dye-Sensitized Solar Cell (DSSC) has been extensively studied due to its easy-to-fabricate, colorful appearance, and transparency with reasonable power conversion efficiency. Many factors can determine the cell's performance, but one of the important determinants is electron transport in TiO_2 films. In this work, we incorporated MWNT into TiO_2 to facilitate the fast electron transport of MWNT. A few previous report claimed that the cell performance can be increased by dispersing MWNT of 0.01 ~ 0.1 wt% in TiO_2 matrix. However, no detailed investigations were performed the effect of MWNT. Rather than simple blending, we synthesized MWNT/TiO_2 to raise the electron transport rate. Cell performances were compared at different MWNT/TiO_2 loadings. Electrical impedance spectroscopy (EIS) was utilized in order to correlate the cell performance to the electrochemical parameters.

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Electrochemical detection of bisphenol A using a tyrosinase-modified biosensor

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Tyrosinase is a binuclear copper containing metalloprotein which catalyses the hydroxylation and oxidation of mono and diphenols to o-quinones. Electrochemistry of tyrosinase was promoted by Au nanoparticle (AuNP)-encapsulated dendrimers (Den), which was applied for the detection of BPA. To increase the electrical properties, AuNPs were captured in the interiors of the dendrimer (Den-AuNPs) as opposed to attachment at the periphery of dendrimer. To prepare Den-AuNPs, the Au(III) ions were first coordinated in the interior of dendrimer with nitrogen ligands and then reduced to form AuNPs. AuNPs-encapsulated dendrimers were then used to covalently immobilize tyrosinase (PDATT/ Den(AuNPs)/ Tyrosinase). CVs show redox peaks at +0.05/ +0.15 V. It was used as analytical signal and obtained the calibration curve with chronoamperometry.

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Elimination of interferences for NADH detection using a LB technique

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An electrochemical sensor for β-nicotinamide adenine dinucleotide (NADH) has been developed. It was constructed using a conducting polymer (5,2´:5´,2´´-terthiophene-3´-carboxylic acid, TTCA) as a base substrate deposited on the screen printed carbon electrode (SPCE) immobilized with Au nanoparticles (AuNPs) and biomaterials including cytochrome c (cyt c), lipids, 1,2-dioleoyl-sn-glycero-3-phosphoethanolamine (DOPE), cardiolipin (CL), and ubiquinone (UQ10). To avoid interference effects, we assembled the lipid bilayer using the Langmuir-Blodgett (LB) technique through controlling the density of the outward lipid layer. The characteristics of modified electrode were investigated by cyclic voltammetry (CV), impedance spectrometry, and quartz crystal microbalance (QCM), and X-ray photoelectron spectroscopy (XPS). The linear response range was observed between 1.0 μM and 5.0 mM NADH concentration at pH 7.0 with a detection limit of 0.5 μM (± 0.15 μM) (S/N = 5). L-ascorbic acid, uric acid, and NADPH did not show any interference during the detection of NADH at the biomimetic lipid bilayer system. The real sample analysis using HT 29 cell line was successfully performed to evaluate the reliability of the proposed sensor.

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Gold Nanoparticle decorated selective detection of anticancer daunomycin by DNA aptasensor

Pranjal Chandra, 노희복, 김동민, 심윤보

부산대 화학과

A DNA Aptamer functionalized sensor probe was prepared by electropolymerization of a conductiong polymer, poly-[2,2':5'2"-terthiophene-3'-(p -benzoic acid)] (poly-TTBA) onto a gold nanoparticle/glassy carbon electrode (AuNP/GCE) and NH2 modified DNA aptamer was covalently bonded to the poly-TTBA through amide bond formation. GCE/AuNP/poly TTBA/DNA aptamer was immerged into 5nm gold nanoparticle solution to fabricate final sensing probe was carried out by employing cyclic voltammetry(CV) and differential pulse voltammetry(DPV). Surface of the electrode was characterized by XPS, QCM, and SEM. Various experimental parameters, pH, temperature, applied potentiall and deposition time were optimized and performance of the daunamycin aptamer sensor was examined. The fabricated aptasensor exhibited a dynamic range of 1.0 x 10-7 and 1.2 x 10-5 M and a detection limit of 2.0 (± 0.01) x 10-8 M (k = 3, n = 5).

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The synthesis and electrochemical properties of Li_2MnO_3

서효리, *이철우, 김건

*고려대 화학과 *성신여대 화학과*

We have been studied the synthesis of the lithium-manganese oxide (Li_2MnO_3) as the positive electrode of lithium ion secondary batteries and compared the electrochemical properties of cathode material according to the synthesis condition. As a manganese source of Li_2MnO_3, we synthesized MnO(OH) at various synthesis temperatures, 100 – 140℃, through hydrothermal reaction and found the condition where MnO(OH) can be formed. To prepare Li_2MnO_3, LiOH•H_2O was mixed with MnO(OH) by solid-state reaction method, and the obtained powder was annealed at 800 and 900℃ for 8 and 4 hours, respectively. Each sample was characterized by x-ray diffraction (XRD), scanning electron microscopy (SEM), and Fourier transform infrared spectroscopy (FT-IR). The electrochemical properties and their charge/discharge behavior was evaluated using the prepared coin cells consisting of Li_2MnO_3 cathode, lithium metal anode, and 1M $LiPF_6$ in DMC/EC (1:1 v/v) electrolyte were investigated.

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Stainless mesh based low-priced and flexible dye-sensitized solar cells

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염료감응형 태양전지의 상용화를 위한 당면 과제로는 크게 세 가지로 낮은 생산단가(Low Cost), 높은 광변환효율(Photon-to-current Conversion Efficiency), 장기안정성(Long Term Stability) 확보에 있다. 본 연구에서는 염료감응 태양전지 제조 공정에서 가장 큰 생산 단가 비중을 차지하는 투명전도성 기판(Transparent Conductive Oxides, TCO)을 대체하기 위해서 광전극층에 금속망(Stainless Steel Mesh)을, 상대전극에 백금이 코팅된 금속포일(Ti Foil)을, 양극간의 단락(Short)을 방지하기 위해서 폴리머 필름(Polymer Film)을 사용하였으며, 금속망에 TiO2 광전극층을 형성시키기 전에 금속망과 전해질 사이에 발생할 수 있는 암전류(Dark Current)를 방지하기 위해서 TiOx 층을 150~200 nm 두께로 진공 증착하였다. 이와 같이 광전극용 금속망을 이용하여 저가이면서 유연한 염료감응 태양전지를 설계 할 수 있었으며, 완성된 태양전지의 광전변환 효율은 □(AM1.5):3.1%, 전류-전압 특성은 Voc:0.58 V, Jsc:11.97 mA/cm2, ff:0.45 로 측정되었다.

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Synthesis and Electrochemical Characteristics of Poly(4-Vinylpyridine)-Osmium-Hyppuric Acid for immunosensor

이예림, 최영봉, 김혁한

단국대 화학과

Urinary hippuric acid (HA), of molecular weight 180 Da, is one of the major metabolites intoluene-exposed humans and is a major biological indicator. Simple and ubiquitous monitoring ofexposure to toluene is very important in occupational health care, and a hydrogel-basedelectrochemical immunoassay for rapid and quantitative detection of HA. The system employs a conjugate of Osmium (Os) and hippuric acid (HA) and then OS-HA reacts with Poly(4-Vinylpyridine) (PVP). The competition between hippuric acid (HA) and PVP-Osmium-HA generated electric signals proportional to HA concentration. The electrochemical immunoassay comprised with immobilization of HA-antibody on the nickel-coated ITO electrode and then apply the mixture HA and PVP-Osmium-HA. The electrical signal was measured by voltammetry technique. The resulting currents were linearly related with the concentration of HA complex. Also the structures of Osmium compounds have been identified by the spectroscopic method.

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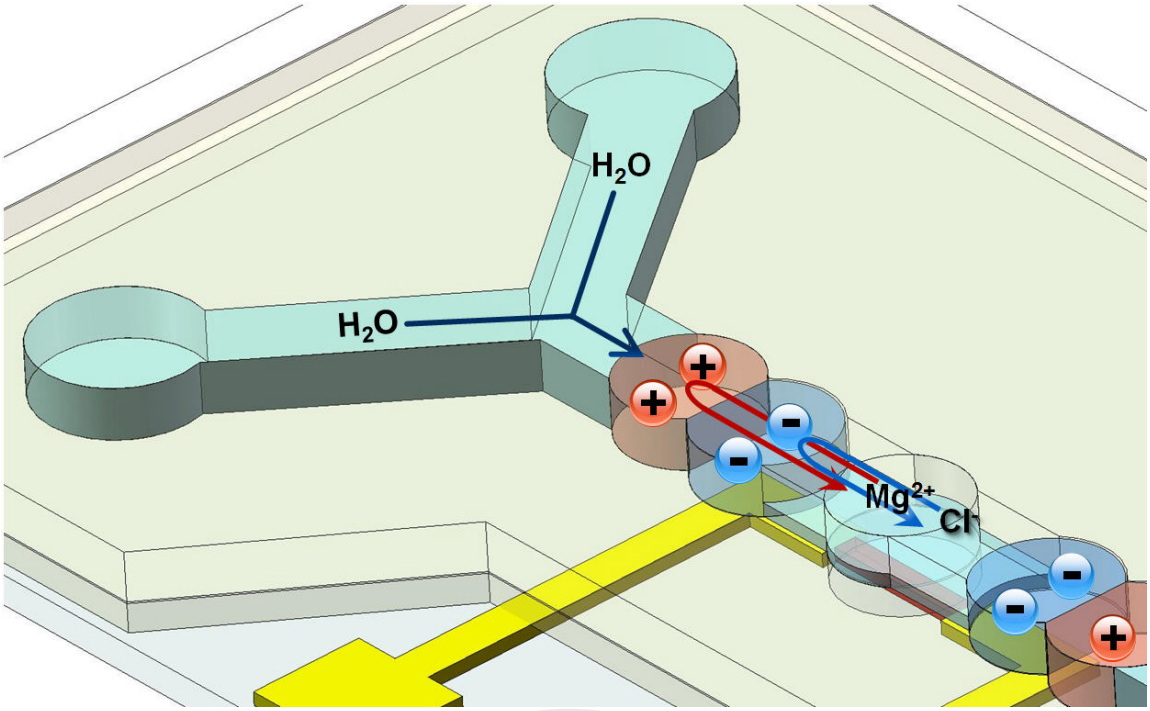
Highly sensitive formaldehyde gas sensor using polyelectrolyte junction.

김지연, 정택동

서울대 화학부

In this paper, we present a gas sensor for formaldehyde by utilizing patterned single-walled carbon nanotube field effect transistors (SWNT-FETs) on a silicon substrate. SWNT-FET is an emerging tool for detecting gas dissolved in aqueous solution since SWNTs have excellent gas absorption ability due to their high surface-to-volume ratio and special electrical properties, such as high carrier mobility and Fermi level shift which is induced by molecular charge transfer. Formaldehyde is a representative harmful gas of the sick building syndrome. In addition, formaldehyde has high solubility in aqueous solution. Therefore, formaldehyde is selected as the target material for the developed gas sensor. Maintaining small volume of aqueous layer is essential for detecting water soluble gas since it helps reducing response time. To achieve this, we fabricated microchannel on poly dimethyl siloxane (PDMS) by casting method and formed photocurable polyelectrolytic gels, which supply water to sensing chamber to keep small volume of aqueous solution. The electrical conductance of the sensor dramatically decreased as the concentration of formaldehyde gas increased. The SWNTs sensor with aqueous layer can detect 0.1ppb formaldehyde at room temperature.



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An amperometric immunosensor based on conjugation of HBs-Ag with mediating metals

최영봉, 김혁한

단국대 화학과

The electrochemical immunoassay system for clinical diagnosis has several advantages such as simple instrumentation, relatively low cost, miniaturization, portability, disposability, and fully automation. The HBs assay system employs a conjugate ferrocene or osmium complexes with HBs-antigen. We have been synthesized HBs-Ag-metal complexes. The series of novel and electro-active HBs-Ag-metal complexes were characterized using electrochemical techniques. The electrochemical immunoassay comprised HBs-Ab-Au nanoparticles and then applied HBs-Ag-metal complex in the micro-tube. The electrical signals were measured by voltammetry technique. The competitive reaction between HBs-Ag and HBs-Ag-metal generated the changes of electrical signal. The resulting currents were linearly related with the concentration of HBs-Ag. A study of the electrochemical immunoassay offers a cheap and portable devices of developing rapid HBs immunoassays.

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Modification of size controlled Pt nanoparticles dispersed on carbon support using spontaneous deposition of Ru toward methanol oxidation

김세철, 김영래, *김잔디, 김혜란, *김혜령, *정창훈, *이충균

*충남대 분석과학기술대학원 *충남대 화학과*

본 연구에서는 Pt 나노입자의 크기에 따른 메탄올 산화와, Ru 비가역 흡착에 의한 메탄올 산화 거동에 대해서 연구하였다. Pt 나노입자는 에틸렌 글리콜을 이용한 폴리올 환원방법과 pH 조절방법을 통해서 1.5 nm ~ 7.5 nm 까지 다양한 크기의 Pt 나노입자를 만들었고, 각각 크기에 따라 제조한 Pt 나노입자에 비가역 흡착 방법을 사용하여 2 mM Ru 과 5 mM Ru 으로 Pt 나노입자 표면을 변형하였다. 메탄올 산화는 반응 표면적이 최대인 1.5 nm 에서 168 A/g 으로 최대 활성을 나타냈다. Ru 에 의한 표면 변형에 따른 메탄올 산화 활성 증가는 두드러지지 않았으나, 메탄올이 산화하기 시작하는 전압(onset potential)은 Pt 나노입자에 비해 0.1 V ~ 0.2 V 정도 환원전위로 이동하는 것을 관찰하였다.

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Observation of a two-dimensional molecular network structure of trimesic acid and dimethylglyoxime by electrochemical scanning tunneling microscope (EC-STM)

김혜란, *김잔디, *정창훈, 김세철, 김영래, **이충균

*충남대 분석과학기술대학원 *충남대 화학과 **충남대 화학과, 분석과학기술대학원*

나노 크기의 3 차원 구조체 형성의 지지체로서 응용하기 위한 2 차원 network 형성을 위해 trimesic acid (TMA)와 dimethylglyoxime (DMG)의 두 가지 분자를 선택하여 electrochemical scanning tunneling microscope (EC-STM)으로 관찰하였다. TMA 는 세 개의 카복실기를 가진 분자로 카복실 그룹에 의한 수소결합을 형성함으로써 안정한 2 차원 network 구조를 형성하는 것으로 잘 알려져 있다. Au(111) 표면에서 TMA 를 전압을 조절하면서 STM 으로 관찰한 결과, 0~200 mV 에서 9×9 의 '2 차원 network' 구조가 관찰되었다. 하지만 200 mV 보다 높은 전압에서는 4×5 의 'closed packed' 구조와 $7\times2\sqrt{3}$ 의 'striped' 구조와 같은 다양한 구조의 2 차원 network 를 관찰하였다. DMG 는 두 개의 카보닐기를 가진 분자로 주로 니켈 이온의 정성 및 정량 분석에 사용되어 왔다. Au(111) 표면에서 DMG 를 전압 조절 없이 STM 으로 관찰한 결과, $2\sqrt{3}\times2\sqrt{3}$ 의 'hexagonal' 구조와 $2\sqrt{3}\times4\sqrt{3}$ 의 'zigzaged' 구조의 두 가지 구조를 관찰할 수 있었다. 이와 같은 DMG 2 차원 network 에 Ni 과 같은 금속 이온을 선택적으로 흡착시켜 석출함으로써 금속 센서나 금속 분리 장치로서 응용할 수 있을 것이다. 선택한 두 분자 모두 2 차원 network 구조를 형성하는 것을 EC-STM 을 이용해 확인 하였으며, 센서나 유기 전자장치 등에 응용하는 기술에 기반이 될 것이다.

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Electrochemical detection of dopamine in the presence of ascorbic acid using graphene modified electrodes

김양래, 김하석

서울대 화학부

Dopamine plays a significant role in the function of human metabolism. It is important to develop sensitive sensor for the determination of dopamine without the interference by ascorbic acid. We report the synthesis of graphene using a modified Hummer's method and its application for the electrochemical detection of dopamine. Electrochemical measurements were performed at glassy carbon electrode modified with graphene via drop-casting method. Cyclic voltammogram of ferri/ferrocyanide redox couple at graphene modified electrode showed an increased current intensity compared with glassy carbon electrode and graphite modified electrode. The decrease of charge transfer resistance was also analyzed by electrochemical impedance spectroscopy. The capacity of graphene modified electrode for selective detection of dopamine was confirmed in a sufficient amount of ascorbic acid (1 mM).

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Enhanced electrogenerated chemiluminescence of the ruthenium tris(2,2')bipyridyl/tripropylamine system on boron-doped diamond nanograss array

양용탁, 김하석

서울대 화학부

The greatly enhanced electrogenerated chemiluminscence (ECL) process of the $Ru(bpy)_3^{2+}$(bpy = 2,2'-bipyridyl)/tripropylamine (TPA) system was achieved on a Boron-doped diamond (BDD) nanograss array which was simply fabricated by reactive ion etching (RIE). This effective enhancement of ECL intensity was attributed to the more facile oxidation of TPA which was arised by the improved electrocatalytic activity and the accelerated the electron transfer. And the hydrophobicity of the electrode surface also plays an important role in the proton-transfer reaction of TPA which takes place in the solution near the surface. As a result, the much larger oxidation rate of neutral TPA and much higher ECL intensity was achieved on the hydrophobic surface. This investigation shows an effective way for the ultrasensitive detection of $Ru(bpy)_3^{2+}$, which may lead to more efficient immunoassay and DNA analysis based on $Ru(bpy)_3^{2+}$ ECL.

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Pd-Co Nanoparticles as Electrocatalysts for Oxygen Reduction

우승희, 김하석

서울대 화학부

Carbon-supported Pd-Co alloy electrocatalysts with different Pd-Co atomic rations were prepared by an improved aqueous impregnation method, in which HCHO was used as a reducing agent and HCl was used as a sedimentation promoter. The prepared catalysts were heated at 300 °C in H_2 (10%) / N_2 (90%) gas for 3hr. A typical TEM image of the Pd_3 Co/C catalyst reveals a mean particle diameter of ca. 3.8 nm with relatively narrow size distribution. An activity evaluation of the oxygen reduction reaction (ORR) on as-prepared Pd-Co/C catalysts with a rotating disk electrode (RDE) technique indicated that the maximum ORR mass activity was obtained when Pd:Co atomic ratio is 3:1. The synthesized Pd-Co/C catalyst exhibits superior tolerance to methanol crossover poisoning than Pt/C.

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Electrochemical Behaviors of Irreversibly Adsorbed Bi on Pt(111) Electrode Surface Studied by Electrochemical Scanning Tunneling Microscopy

정창훈, 김잔디, 이충균

충남대 화학과

본 연구는 개미산 산화에 있어 Pt 전극의 촉매 활성을 증가시키는 외부 금속으로서 사용되는 Bi 의 전기화학적 거동을 원자 수준에서 이해하고자 하는 데 있다. 본 연구를 위해 cyclic voltammetry 와 electrochemical scanning tunneling microscopy (STM)가 사용되었다. Bi 의 비가역흡착은 0.5 M H^2SO^4 에 포화된 Bi 용액에 Pt(111) 전극을 접촉하여 수행되었다. Pt(111) 전극 표면에 비기역적으로 흡착된 Bi 의 덮힘률과 표면 형상은 Pt(111) 전극과 Bi 용액과의 접촉시간에 의해 결정된다. 최대 Bi 덮힘률은 60 초 동안 비가역 흡착에 의해 얻어졌다. 10 초, 30 초, 60 초 동안 Bi 의 비가역 흡착 후, Pt(111) 표면에 형성된 Bi 흡착층은 island, monolayer, second-monolayer 형태로 형성됨이 관찰되었다. 열린회로전압에서, Pt(111) 표면에 형성된 산화종 Bi 흡착층의 원자 구조는 ($\sqrt{2} \times 2\sqrt{2}$) 구조이었으며, Bi 의 환원, 재 산화 과정에 의해 Bi 의 흡착 구조는 변화되지 않는 것으로 관찰되었다. 다만, Bi 의 환원과 재 산화 과정에 의해 Bi 원자 배열 사이에 산소원자의 삽입과 탈착이 이루어 지는 것으로 해석되었다.본 연구는 기존에 보고되었던 Pt(111) 표면에서 Bi 의 비가역 흡착에 의한 의 흡착구조 및 흡착층의 형상등에 대한 연구 내용 잘못된 것임을 밝히고, 본 연구를 통해 얻어진 새로운 결과를 보고한다.

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Surface Characterization of Pulsed-Plasma Polymerized Fluorocarbon Thin Films

이지혜, 김강진, *이연희

*고려대 화학과 *KIST 특성분석센터*

Plasma polymerization is a thin film deposition process and can be uniformly coated onto the substrate. Plasma polymers generally have different properties from those of conventional polymers due to their unique properties. Plasma polymer films have been used in a variety of applications including barrier coating, protective coating, and anti-scratching coating. In this study, plasma polymerized films fabricated by pulsed plasma. We used three kinds of fluorine-containing gases such as C_2F_6, C_3F_8, and C_4F_8. Process parameters for plasma polymerization such as gas ratio, gas pressure, plasma power, pulse frequency, and processing time were investigated. Surface analytical instruments such as Auger Electron Spectroscopy (AES), X-ray Photoelectron Spectroscopy (XPS), and Time-of-Flight Secondary Ion Mass Spectrometry (TOF-SIMS) were used to provide useful information about the chemical properties such as surface composition and functional groups. And, film thickness and surface morphology were also observed using Field-Emission Scanning Electron Microscope (FE-SEM) and Atomic Force Microscope (AFM).

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Development of a Disposable OSCS Detector based on a Potentiometric Polyion-sensitive Electrode

권기학, 강영재, 신재호, 남학현, 차근식

광운대 화학과

Heparin is widely used as an injectable anticoagulant. In March, 2008, the FDA identified oversulfated chondroitin sulfate (OSCS) as a contaminant in heparin originating from China. Because of the similarities in chemical structure and anticoagulant activity, it is difficult to detect OSCS in the pure heparin. A very simple and inexpensive method to detect oversulfatedchondroitin sulfate (OSCS) or other high-charge density polyanionic structures as contaminants in heparin products using potentiometric polyanion sensors is described. In the potentiometric measurement, a greater change in the phase boundary potential of polymeric membranes formulated with tridodecylmethylammonium (TDMA) anion exchange sites is observed for the contaminated heparin than for the pure heparin due to the higher charge density of OSCS or other impurities compared to that of porcine heparin. Our proposed electrochemical sensor is much more simple, easy to use, fast, and cost efficient than conventional NMR and CE methods. The detection limit of the NMR analysis is known to be 0.1 wt% OSCS in 57 mg/mL heparin sample. In our approach, the detection of 0.007 wt% OSCS impurity is readily achieved with the same heparin sample with high reproducibility. Even lower detection limits for OSCS contamination is currently pursued.

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Ammonium ion-selective electrodes fabricated with self-assembled monolayers of ionophoric receptors based on the ion-channel mechanism

진선민, *이재선, *강영재, *신재호, *차근식, *남학현, **Aasif Helal, **김홍석

*광운대 화학과 *광운대 화학과 **경북대 응용화학과*

Self-assembled monolayers (SAM's) with thiozole-benzo-crown ether-ethylamine (TBCEA)-thioctic acid on polycrystalline gold disk electrodes are investigated for the selective ammonium detection in the aqueous solution. The voltammetric ion-channel sensing is a well-known technology where the specific adsorption of analyte on the SAM-modified electrode significantly modulates the electron transfer rate of the redox species such as $[Ru(NH_3)_6]^{2+/3+}$. In the initial study of SAM only with the ammonium ionophore (i.e., TBCEA-thioctic acid), the ion-channel mechanism with the redox markers did not exhibit the sufficient concentration-dependent response for ammonium cation. Further optimizations were conducted by employing mixed SAM's with various thiol moieties. Significant ammonium-dependent response is observed when the hydrophobic alkyl thiol is included in the mixed SAM's in order to mimic the configuration of the plasticized polymeric membrane. The selectivity pattern of the mixed SAM-based ion-channel sensor is compared with that of the conventional ion-selective electrode based on the plasticized poly(vinyl chloride) (PVC) membrane containing the TBCEA-thioctic acid. Various ratios of the alkyl thiol and ionophore were investigated to examine the role of alkyl thiols self-assembled with TBCEA-thioctic acid. The impedance study was also conducted to probe the electrostatic repulsion behavior of the electrode surface for the redox couple depending on various concentrations of ammonium. Furthermore, we observed the quasi-reversible adsorption/desorption of ammonium depending on concentration of the solution, which caused the quasi-reversible electrostatic repulsion of positively charged $[Ru(NH_3)_6]^{2+/3+}$.

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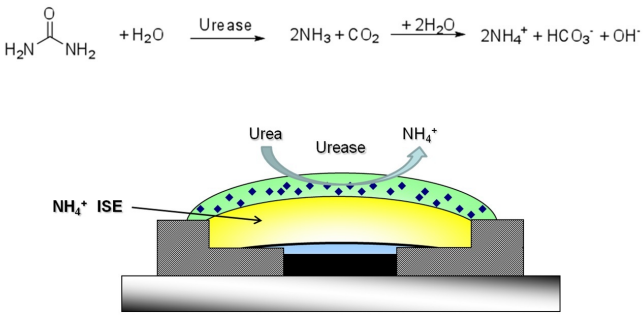
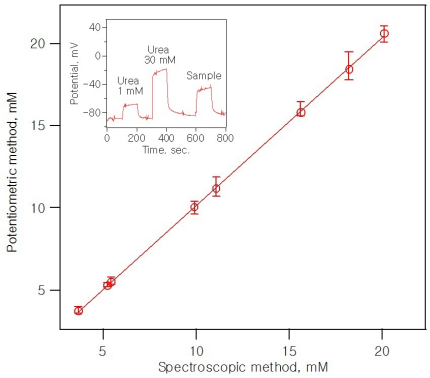
A disposable biosensor for the determination of urea in physiological fluids

허민, 이재선, 김영국, 차근식, 남학현, 신재호

광운대 화학과

The level of urea in serum and whole blood is a reliable indicator of the renal failure. A normal concentration of urea in serum is typically ranged from 2.5 to 7.5 mM. However, the patients with the urea concentration above 30 mM are considered to have the renal failure, eventually requiring hemodialysis. Several approaches have been developed to determine the urea concentration in physiological fluids, including most commonly colorimetric and spectrometric methods. The utility of such methods has been, unfortunately, limited due to tedious, complicated sample pretreatment processes. However, the urea biosensor based on the ammonium ion-selective electrode (ISE) takes advantages of fast response time, ease to miniaturize, and no sample pretreatment. Despite unique benefits of using potentiometric urea biosensors, its applicability in miniaturized and disposable-type sensing systems has been restricted because of relatively long preconditioning time. Herein a saturated NaCl layer is introduced as internal electrolyte medium for the ammonium ISE to reduce sensor's preconditioning time. One-point and two-point calibration methods are evaluated to precisely determine urea concentrations in physiological fluids (e.g., serum and whole blood). Finally, the clinical performance of the resulting urea biosensors will be compared to that of a bench-top spectroscopic system (Vitros DT60 II).





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발표분야: 전기화학
발표종류: 포스터, 발표일시: 목 15:00~17:00

Development of Amperometric Microsensors for the Detection of Signaling Gas Molecules *in Vivo*

박선아, 박선아, *이영미, *이영미, *이영미

*이화여대 화학 나노과학과 *이화여대 자연과학대학/화학전공*

Nitric oxide (NO) is well known for its crucial physiological functions as a vasodilator, a neurotransmitter, a mediator of anti-tumor activities, etc. In addition, there are other important signaling gas molecules functioning similarly to NO. It is of great interest to measure two different gas molecules in biological systems. Therefore, we developed a novel amperometric microsensor and tested its feasibility by applying the sensor for *in vivo* real-time measurements of these signaling molecules. The developed microsensor is composed of a planar microdisk working electrode and a Ag/AgCl reference electrode immersed in an optimized internal solution covered with permselective gas-permeable membrane for the selectivity to gas only. The working electrode potentials, the internal solution compositions, and the sensor dimension are optimized to improve the sensor performance. This research was supported by “Systems Biology Infrastructure Establishment Grant” from the Gwangju Institute of Science and Technology.

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발표종류: 포스터, 발표일시: 목 15:00~17:00

Heterogeneity of Skin Oxygen Density Distribution: Relation to Location of Acupuncture Points

장경, *이영미

*이화여대 화학 나노과학과 *이화여대 자연과학대학/화학전공*

To investigate possible functions of acupuncture, oxygen (O_2) levels were measured at two different acupuncture points (APs) [Hegu and Laogong] and at the corresponding non-APs (3-5 cm away from the APs) in real time using a high sensitive electrochemical O_2 microsensor. The sensor had a small planar sensing platinum disk (diameter=25 μm) and therefore was able to monitor the O_2 levels at the localized APs. Significantly higher O_2 levels (*pn*=5, without exceptions) in comparison with the non-APs. Sufficient sensor sensitivity to distinguish the O_2 level differences between APs and non-APs was achieved. This research provides useful information on possible functions of APs and meridians. This research was supported by “Systems Biology Infrastructure Establishment Grant” from the Gwangju Institute of Science and Technology.

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발표종류: 포스터, 발표일시: 목 15:00~17:00

Electrocatalytic Effects of Activated-Gold Electrodes in Neutral Aqueous Media

김지영, *심준호, **이종목, ***이영미

*이화여대 나노화학과 *이화여대 신재생에너지연구센터 **이화여대 화학과 ***이화여대 자연과학대학/화학전공*

An electrocatalytic cathodic reduction of molecular oxygen for the fuel cell development was investigated on bulk Au and Au nanoparticle-modified glassy carbon (AuNP/GC) electrodes, respectively, in the presence and absence of the electrochemical pretreatment process in a neutral oxygen-saturated phosphate buffer solution. From rotating disk electrode voltammetric experiments, it was found that the preactivated bulk Au and AuNP/GC electrodes exhibited a largely low cathodic overpotential and a highly increased current density when compared with corresponding non-pretreated ones. To confirm our understanding of the effects of electrochemical treatment, thermally treated gold wire for the oxygen reduction reaction (ORR) was also investigated in neutral aqueous media. In addition, we examined the electrocatalytic activity of these electrodes for the electrochemical reduction/oxidation of hydrogen peroxide, which is an enzymatic intermediate substance of many enzyme-substrate reactions. The result revealed quite similar tendency to the one obtained for ORR. This research was carried out under the General R/D Program of the Daegu Gyeongbuk Institute of Science & Technology (DGIST), funded by MEST, ROK.

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발표종류: 포스터, 발표일시: 목 15:00~17:00

Characterization of the Activity of Porous Metallic Electrocatalysts for Oxygen Reduction Reaction Using Scanning Electrochemical Microscopy

양지혜, *이영미, **이종목

*이화여대 화학나노과학전공 *이화여대 자연과학대학/화학전공 **이화여대 화학과*

Due to the high cost and the limited supply of Pt, which shows generally the best activity for sluggish oxygen reduction reaction (ORR) in polymer electrolyte membrane fuel cells (PEMFC), extensive research has been performed to search alternative economic and efficient electrocatalytic materials. Therefore, we prepare a variety of porous metallic electrocatalysts by simple electrodeposition with or without controlling the microstructures called mesoporous structures. In addition to Pt (for comparison), Pd is electrodeposited on a platinum microdisk substrate. The location-dependent ORR activities of the prepared porous metallic electrocatalysts (mesoporous or not structure-controlled) are studied by scanning a small Pt-disk tip electrode using scanning electrochemical microscopy (SECM) in tip generation–substrate collection (TG-SC) mode: O_2 generated at the tip is reduced at the electrocatalyst substrate. Potential dependency of the catalyst ORR activity is also examined by rotating disk electrode experiments. The study of morphologies of the electrocatalysts are also obtained using SECM in TG-SC mode in a solution of reversible electroactive species ($Ru(NH_3)_6^{3+}$): $Ru(NH_3)_6^{3+}$ is reduced to $Ru(NH_3)_6^{2+}$ at the tip surface and then the produced $Ru(NH_3)_6^{2+}$ is oxidized at electrocatalyst substrate . The observed morphology and the local ORR activity of the electrocatalysts are compared and analyzed. This research was carried out under the General R/D Program of the Daegu Gyeongbuk Institute of Science & Technology (DGIST), funded by Ministry of Education, Science and Technology (MEST) of the Republic of Korea.

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발표종류: 포스터, 발표일시: 목 15:00~17:00

Electrochemical Gas Microsensors Based on Pore-Type Working Electrodes

도현경, *이영미

*이화여대 화학나노과학 *이화여대 자연과학대학/화학전공*

Over the last two decades, the demand for improved electrochemical sensors suitable for biological applications has been significantly increased. In particular, the use of electrochemical sensor with small sensing dimension (micro- to submicro-meters) would allow the location-dependent measurements of biological analytes of our interest. In this presentation, we will show the development of a novel amperometric gas sensor based on a pore-type working electrode intended to detect important biological gas molecules. The senor is fabricated as follows: (1) a microdisk electrode is prepared by polishing an etched Pt in a glass capillary; (2) the microdisk Pt is further etched to produce a conical pore; (3) chemical modification is applied on the pore electrode for the sensor selectivity to gas molecules only; (4) Pt base surface in the pore electrode is electrochemically modified to improve sensor sensitivity. The feasibility of the developed sensors is tested by calibration procedures. The sensitivities were obtained in between each fabrication step. This research was supported by “Systems Biology Infrastructure Establishment Grant” from the Gwangju Institute of Science and Technology.

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발표종류: 포스터, 발표일시: 목 15:00~17:00

Simultaneous Determination of Hydroquinone and Catechol at anActivated Glassy Carbon Electrode

Ahammad A.J Saleh, *이재준

*건국대 신소재공학과 *건국대 응용화학과*

A selective and very simple electrochemical method, based on anodization of a glassy carbon electrode (GCE), was developed for the simultaneous detection of hydroquinone (HQ) and catechol (CT). It was found that the activated GCE showed an excellent catalytic behavior and enhanced reversibility towards the oxidation of both HQ and CT.The redox responses from the mixture of HQ and CT were easily resolved at an activated GCE. The detection limits for HQ and CT were calculated to be 0.16 and 0.11 μM, respectively. The activated GCE was successfully examined for real sample analysis with tap water and it showed a stable and reliable recovery data.

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Label-Free DNA hybridization detection by the perturbation of charge transfer through DNA at poly (thionine) modified GC and Gold electrode

Md.Mahbubur Rahman

건국대 신기술융합학과

We report three different types of simple and label-free electrochemical sensor for recognition of the DNA hybridization based on the conducting polymer, poly (thionine). Thionine precursor can be easily electrochemically deposited onto the electrode surface in different pH medium. It showed a high electrochemical sensitivity in aqueous medium. Pendant amino group of the polymer surface was covalently grafted with the ss-DNA probe and it was tested by hybridization with complementary DNA segments. Differential pulse Voltammogram (DPV) showed a decrease of the oxidation current of [Fe (CN) 6] 3-/4- upon immobilization of ss-DNA probe. It was further decreased upon hybridization of the complementary DNA. Electrochemical impedance spectroscopy (EIS) indicated the increase of the charge transfer resistance (Rct) and also the decrease of the charge transfer rate constant (Kao) after hybridization. It suggested that the DNA duplex formed an obstacle against the ion movement of the redox couple. These results are in good agreement with those obtained by differential pulse voltammetry (DPV). The three different type of PTH modification (one step PTHGC, two steps PTHGC and PTHGold) were compared and they showed a reliable selectivity and sensitivity for the sensing the DNA hybridization. Complementary DNA sequence as low as 1pM could be detected with these three different types of transducers. It suggested that a practical, label-free, and real-time sensor can be constructed with PTH-modified electrodes.

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Cathodic Stripping Voltammetric Determination of Tellurium(Ⅳ) using a Bismuth Film Electrode

함선영, *최승언, *채유진, *김환기, 팽기정, *명노승

*연세대 화학과 *건국대 응용화학과*

기존 Hg 전극을 대체할 수 있는 Bi film 전극을 이용하여 Te4+ ion 의 정량분석법을 개발하였다. Glassy carbon 전극 표면에 Bi(NO3)3 용액을 이용하여 가장 적합한 film 의 두께를 결정한 뒤 Te 표준용액과 Bi film 전극을 이용하여 각각의 원소에 대한 검량선, 검출한계, 정밀도 등을 얻었고, 몇몇 중금속(Cu2+, Cd2+, Se4+)들의 방해효과도 연구하였다. Bi film 과 Te 의 반응 시 Te 뿐만 아니라 Bi2Te3 와 같은 화합물들이 생성되는지 알아보고, Bi2Te3 화합물이 생성될 때 Bi film 전극의 표면에서 일어나는 Bi 화합물(Bi2Te3)의 전기화학적 현상도 규명하였다. Stripping analysis 에서 사용되어 왔던 Hg film 을 이용하여 Te 을 정량분석 하였고, 그 결과를 Bi film 전극을 이용하여 얻은 결과와 비교 분석하였다.

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발표종류: 포스터, 발표일시: 목 15:00~17:00

Electrochemical desorption of organc layers from various electrode surfaces

Al-Monsur Jiaul Haque, 강현주, 김규원

인천대 화학과

This presentation reports electrochemically reductive and oxidative desorption of organic layers on various electrode surfaces, which have been used for the immobilization of biomolecules. The organic layers were prepared by electrochemically reductive depositon of aryldiazonium salts. The diazonium salt modified electrodes have been known that it is highly stable and shows good performance for sensor application. Cyclic voltammetry and X-ray photoelectron spectroscopy have been employed for the characterization and comparison of the electrode surfaces before and after desorption reaction for each electrode. We also demonstrates a multiplex biosensor application based on the electrochemical desorption.

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발표종류: 포스터, 발표일시: 목 15:00~17:00

A Novel Synthesis Approach of Supported Pd/VC Catalysts for Proton Exchange Membrane Fuel Cell

김민식, 김정호, *Nitin Chaudhari, *kiran chaudhari, *김민우, *임신묵, *송민영, **양대수, 유종성

*고려대 신소재화학과 *고려대 소재화학과 **고려대 신소재화학*

A highly efficient homogenous deposition (HD) approach was employed to synthesize commercial Vulcan carbon (VC)-supported Pd (60 wt%) catalysts by varying the amount of urea. In this method, urea was used to generate in-situ hydroxide ions upon hydrolysis at elevated temperature, resulting in an even increase of pH in the whole solution and homogeneous deposition of Pd species on the VC support. In addition, it was found that the urea amount in the staring solution has significant influence on the Pd metal particle size and the catalytic activity of the supported Pd catalyst. Several variations were investigated for the amount of urea to be used. Almost all of the variations led to smaller metal particle size and better particle dispersion on the support. Compared with the Pd catalyst prepared by the impregnation-NaBH4 method at pH 7~8, the catalyst synthesized by HD method demonstrates greatly improved catalytic performance in proton exchange membrane fuel cell. Furthermore, this method is extremely simple and straightforward. The results presented in this study highlight that urea-assisted HD approach is highly efficient for synthesis of supported catalyst with high metal loading.

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발표종류: 포스터, 발표일시: 목 15:00~17:00

Development of screen printed and gold microarray immunosensors based on impedance measurements for the detection of IgG

최지혜, *박혜준, **박덕수, ***장승철

*부산대 분자화학기술협동과정 *부산대 분자과학기술협동과정 **부산대 바이오피지오연구소*
****부산대 바이오피지오센서기술연구소*

This poster describes the development of an electrochemical immunosensor for the measurement of IgG. In order to construct electrodes two types of interdigitated electrodes were fabricated: 1) screen-printed carbon ink electrodes printed on a PVC substrate and 2) gold deposited micro array electrodes on a glass substrate. All electrodes 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 non-competitive sandwich immunoassay format, this allowed the ratio of initial to final electrode capacitance to be directly linked with 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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발표종류: 포스터, 발표일시: 목 15:00~17:00

Alizarin Red S modified screen printed carbon electrodes for the amperometric detection of aluminum Ion

박혜준, *최지혜, **장승철, ***박덕수

*부산대 분자과학기술협동과정 *부산대 분자화학기술협동과정 **부산대 바이오피지오센서기술연구소 ***부산대 바이오피지오연구소*

Alizarin Red S modified screen printed carbon electrodes were developed for a rapid, sensitive and specific technique for the electrochemical detection of aluminum ion in water samples. The electrodes developed use screen-printed carbon electrodes (SPCEs) coupled with chemical modification with an organic chelator, Alizarin Red S (ARS), for aluminum ion detection in aqueous solution. The electrochemical detection of aluminum was carried out based on the measurement of changes in the electrochemical behavior of the chelator upon complexation with the aluminum ion. For sensor fabrication ARS was directly immobilized on the surface of SPCEs using a hydrogel, poly(vinyl alcohol) bearing stryrylpyridinium groups (PVA-SbQ). Aluminum concentrations were indirectly estimated by amperometric determination of the remaining non-complexed ARS immobilized on the electrodes, after its complexation with aluminum. The sensitivity of the sensor developed was 3.8nAmM-1cm-2 and the detection limit for aluminum was 11mM.

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발표종류: 포스터, 발표일시: 목 15:00~17:00

Effect of cathodic biofilm on the performance of air-cathode single chamber microbial fuel cells

Ahmed Jalal, 김성현

건국대 특성화학부 생명공학과

Biofilm is inevitable in a bioelectrochemical system (BES) with microorganism as a sole biocatalyst. Cathodic biofilm (CBF) work as a double edges sword in the performance of the air-cathode microbial fuel cell (MFC). Proton and oxygen crossover through the CBF are limited by the robust structure of extracellular polymeric substances (EPS) and composition of available environmental constituent from which the biofilm formed. MFC performance in terms of power, current and coulombic efficiency is greatly influenced by the nature and origin of CBF. Controlled formations of CBF from different ecological environment while keeping same anode inoculums, contribute different magnitude of resistance in the total internal resistance manipulating the overall MFC performance and coulomb efficiency. This study demonstrates that, MFC operation condition can be optimized on the choice of initial substrate that leads to the biofilm formation on the air cathode.

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발표분야: 초중등교사・화학교육
발표종류: 포스터, 발표일시: 금 10:30~12:30

중학교 화학교과에 있어 사고실험이 실험수업을 대체할 경우학업 성취도에 미치는 영향

하동수, 이강범, *박종근

*순천대 화학교육과 *경상대 화학교육과*

현재 교육과정의 제한된 수업시수에 모든 실험을 직접 다룰 수 없다. 따라서 실험수업만을 강조 할 수 없는 것이 현실이다. 여러 제한된 조건들로 인해 이루어지기 어려운 실험수업의 대안으로 시간이나 자료준비 등의 측면에서 교사의 부담을 크게 줄여주면서 탐구적 수업의 진행이 사고실험으로 대체될 수 있다고 가정해 보았다. 이에 따라 수업을 사고실험으로 진행하여 중학교 화학 단원의 성취도 분석을 해보고자 한다. 또한 직접 실험을 해서 얻은 학습효과와 유의미한 차이가 발생하는지를 통해 직접 실험수업의 대안으로 사고실험의 가치가 있는지 알아보고자 한다.

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발표종류: 포스터, 발표일시: 금 10:30~12:30

영·호남 6개대학 부설 과학영재교육원중등화학 강의교재 제목 비교·분석

하동수, 이강범, *박종근

*순천대 화학교육과 *경상대 화학교육과*

영·호남 6 개대학 부설 과학영재교육원의 중등화학 강의교재의 제목을 비교·분석하였다. 과학영재교육원 중등화학 기초·심화과정 교육 프로그램 분석에서 도출된 문제점 분석은 "영재들에 대한 효과적인 영재성 개발"과 같은 영재교육 목표를 실천하는데 저해되는 요소들을 제거하고, 보다 효율적 목표를 제시하는데 있다. 또한,문제점 분석은 다른 영재교육 기관이나, 수학과 같은 다른 과목의 영재교육 프로그램에도 큰 영향을 줄 수 있다. 또 일반 초·중등학교의 화학교육 과정에서, 우수한 학생들의 창의력이나 사고력 향상과 관련된 문제점을 해결할 수 있는 교육 프로그램을 개발하는 데 기여할 수 있다.

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발표종류: 포스터, 발표일시: 금 10:30~12:30

7차 교육과정에 따른 고등학교 화학Ⅱ STS 교육내용 분석

하동수, 이강범, *박종근

*순천대 화학교육과 *경상대 화학교육과*

고등학교 화학 Ⅱ 8 종의 교과서의 STS 내용의 포함 정도 및 각 단원에 얼마나 포함되었는가를 분석하였고, Yager 가 제시한 'STS 교육과정의 필수구성요소'와 Piel 이 제시한 'STS 주제영역', SATIS 프로그램을 기준으로 STS 교수 활동영역을 교과서별 각 항목별로 나누어 분석하였다.

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묽은 용액의 성질에 대한 예비교사들의 이해 및 교사교육과정에 대한 인식

이송연, 백성혜

한국교원대 화학교육과

이 연구는 화학 전공 예비교사를 대상으로 하여 그들이 받고 있는 예비 교사 교육과정을 살펴보았다. 예비 교사 교육과정에 대한 조사가 사범대학을 중심으로 이루어지고 있으며, 교사를 양성하는 다른 제도인 비사범대학 교직이수 과정 중의 예비교사에 대한 연구가 미흡하였으므로, 이 연구에서는 사범대학과 자연대의 교직 이수를 한 예비교사들을 대상으로 심층적인 비교 연구를 수행하였다. 또한 7 차 교육과정에서 다루는 과학 개념 중에서 학생들에게 매우 어렵다고 밝혀진 '묽은 용액의 성질'을 소재로 하여 고등학교 화학Ⅱ 교과서 및 대학 교재를 분석하고, 예비교사들의 사고를 알아보았다. 연구 결과, 다루는 교재나 내용면에서 사범대학과 비사범대학은 큰 차이가 없었고 묽은 용액에 대한 이해에 학교별 차이가 없는 것으로 보아 교과교육학의 강좌수의 차이나 전공 화학 강좌수의 차이가 예비교사들의 이해에 영향을 미치지 못한 것으로 보인다. 그러나 자연대 학생들은 교과교육학과 실습 기간의 이수학점이 사범대 학생들 보다 적기 때문에 이러한 문제가 생긴다고 생각하였고, 반면 사범대 학생들은 화학 내용에 대한 실천적 지식이 부족하기 때문이라고 생각하였다. 이 연구 결과를 통해 예비교사들의 실천적 지식향상을 도모할 수 있는 방향에 대해 모색해 보고자 한다.

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중등 과학영재 수업에서 SSC(Small-Scale Chemistry)실험의 적용 효과

유미현

아주대 교육대학원

SSC(Small-Scale Chemistry)는 비전통적인 화학 실험기구를 사용하여 실험하는 새로운 화학 실험 방법으로 환경적, 경제적 측면에서 여러 가지 장점을 가지고 있는 획기적인 실험 방법이다. 특히 SSC 실험에서 사용하는 기구들은 다양한 실험에 창의적으로 응용될 수 있다. 이미 여러 선행연구들에서 SSC 를 활용한 화학 실험 수업이 일반 학생의 과학성취도, 학업적 자기효능감, 과학탐구능력, 과학적 태도를 향상시키는데 긍정적인 효과가 있음을 보고하고 있다. 그러나 SSC 실험을 과학영재 수업에 적용하였을 때 얻을 수 있는 효과에 관한 연구는 보고된 바가 없다. 본 연구에서는 경기도의 대학부설 과학영재교육원에 선발되어 교육받고 있는 중등과학영재 학생을 대상으로 SSC 실험 수업을 5 차시 실시한 후 SSC 실험이 과학영재의 문제 발견능력, 과학탐구능력, 창의적 사고 등에 미치는 효과를 조사하였다. 그 결과에 따른 교육적 함의를 분석하였다.

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초등 현직 및 예비 교사의 새로운 초등학교 3,4학년 과학 교과서에 실린 화학 영역에 대한 인식 조사

공영태

진주교육대 과학교육과

새로운 과학교육과정이 2007 년에 개정되어 2010 년 3 월부터 새로운 과학교육과정이 초등학교 3,4 학년을 대상으로 적용되었다. 이에 맞추어 기존 과학 교과서와 외형적으로 차별화된 새로운 과학 교과서가 발행 사용되고 있다. 초등학교 3 학년에 '나노 튜브' 관련 내용이 포함되고, 종전의 4 학년에서 학습하는 내용이 3 학년으로 이행 통합되는 등 종전의 학습 내용보다 고도한 학습 내용이 많아졌다고 할 수 있다.이번 연구에서는 현직 교사 100 명과 예비 초등 교사 100 여명을 대상으로 하여 이들의 새로운 초등학교 3,4 학년 과학 교과서에 실린 화학 영역에 관한 인식 조사를 통하여 교사들의 이해도 및 수업에 관한 자신감 등의 정의적 측면을 살펴보고 새로운 과학교육과정의 성공적인 적용을 위한 기초적인 자료를 얻는데 목적을 두었다.

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발표종류: 포스터, 발표일시: 금 10:30~12:30

교과서 국제 비교 (I) -이온 학습 시기의 적절성-

공영태

진주교육대 과학교육과

새로운 중학교 과학교육과정이 2007 년 12 월에 개정 공표되었다. 이 가운데 가장 커다란 특징으로는 현행 교육과정에서 고등학교로 이행되어진 '이온'관련 내용이 다시 부활된 것이다. '이온'관련 개념의 삭제에 대한 현장 교사들의 불만이 개정 직후부터 줄곧 제기되었고 이번 개정에서는 이들의 목소리를 반영한 결과로 생각된다. 하지만, 현행 교육과정에서 '이온'개념이 삭제된 이유도 불분명하고, 또한 이번 개정에서 다시 도입된 이유 또한 불분명하다. 이번 연구에서는 이를 뒷받침하기 위한 자료적인 근거를 찾기 위하여, 국제사회에서의 이온 개념의 학습 내용과 학습이수시기에 대하여 문헌적 고찰을 행하였다. 12 개국 20 개 교과서에 실린 이온 개념에 대한 학습 내용과 이수시기를 고찰하여, 중학교 과학교육과정에서 이온개념의 교수학습에 도움이 되는 시사점을 찾고자 하는데 목적을 두었다.

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인터넷 게시판의 화학 교사 Q&A 분석

이재연, *한재영

*충북대 화학교육과 *충북대 사범대학 화학교육과*

화학 교사는 화학이라는 학문에서 연구되고 발달된 지식, 탐구, 태도 등을 학생들에게 제시하여 교육하는 일을 담당한다. 학생들에게 화학을 가르치면서 미래의 화학자를 길러내기도 하고 미래의 일반 시민으로서 화학적 교양을 심어주기도 한다. 이를 위해 화학 교사는 화학의 내용(지식)이나 방법(탐구) 등에 스스로 익숙해져야 할 뿐 아니라, 그것을 효과적으로 제시하는 방법을 개발하는 데 끊임없이 노력을 해야 한다. 이 과정에서 화학 교사는 잘 모르거나 확신하지 못하는 내용(방법)에 접하게 되는 경우가 종종 있다. 이를 해결하기 위해 주위의 사람들과 질의-응답을 하는 대표적인 통로로 인터넷 Q&A 게시판을 들 수 있다. 화학 교사들이 질문을 올리고 대답을 하는 Q&A 게시판 두 곳에 올라온 내용을 분석하였다. 이 연구의 결과는 예비 및 초임 화학 교사 교육에 유용하게 활용될 수 있을 것이다.

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화학을 공부하는 학생들의 Q&A 분석

지윤정, *한재영

*충북대 화학교육학과 *충북대 사범대학 화학교육과*

초등학교와 중학교, 고등학교 및 대학교에서 많은 학생들이 화학(과학)을 공부하고 있다. 성인 화학자나 일반인은 모두 학창 시절에 (어려운!) 화학을 공부해 본 경험을 가지고 있을 것이다. 학문적 연구를 하는 화학자나 화학을 가르치는 화학 교사는 화학 공부에 어느 정도 성공한 사람들이다. 하지만, 대부분의 학문이 그렇듯이, 화학을 전공하지 않은 사람들에게는 화학이 매우 어렵고 궁금한 점이 종종 생기게 마련이다. 화학을 공부하는 학생의 입장에서 어떤 도움이 필요한지, 어떤 화학 내용이 어려운지에 대한 정보를 얻기 위해 인터넷 Q&A 게시판에 올라온 화학 관련 질의-응답 내용을 분석하였다. 화학에 익숙하지 않은 학생들이 어려워하는 분야와 내용을 조사함으로써, 미래의 효율적인 화학교육 방안 도출에 시사점을 얻는다.

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발표종류: 포스터, 발표일시: 금 10:30~12:30

초등학생의 학습접근양식에 따른 비유만들기 특성과 대응 관계 이해도, 대응오류 및 인식 조사

강훈식, *천지현

*춘천교육대 과학교육과 *강릉 옥천초등학교*

이 연구에서는 '거름종이를 이용한 혼합물의 분리' 원리에 대해 초등학생들이 만든 비유의 특성과 대응 관계 이해도 및 대응 오류 유형, 비유 만들기에 대한 학생들의 인식을 조사하였다. 또한, 학습접근양식에 따라 그 결과가 다른지도 조사하였다. 이를 위해, 강원도 소재 초등학교 4 학년 92 명을 선정하여 사전 검사로 학습접근양식 검사를 실시한 후, 비유 만들기에 대한 오리엔테이션을 실시하였다. 그 후, 비유 만들기 검사와 비유 만들기에 대한 인식 검사를 실시하였다. 연구 결과, 기계적 학습접근양식을 지닌 학생들보다 유의미 학습접근양식을 지닌 학생들이 더 많은 수의 비유를 만드는 것으로 나타났다. 만든 비유 유형의 경우, 표현 방식(글, 그림, 글/그림)과 상황의 작위성(작위적, 일상적), 추상도(추상적, 구체적) 항목에서는 학습접근양식에 따른 차이가 거의 없었다. 그러나 유의미 학습접근양식을 지닌 학생들이 비유와 목표 개념의 속성이 구조적 속성과 기능적 속성을 모두 공유하는 '구조적/기능적 비유', 공유된 속성에 대한 부연 설명이나 비유의 제한점에 대한 설명을 제시하는 '부연 비유', 목표물의 인과 관계에 대응되는 구조를 체계적으로 포함한 '고체계성 비유'를 더 많이 만드는 경향이 있었다. 또한, 유의미 학습접근양식을 지닌 학생들이 비유에 대한 이해도가 높아 적절한 비유를 선택하는 경우가 더 많았고, 자신이 만든 비유에 대한 대응 관계 이해도도 높아 대응 오류를 범하는 경우도 상대적으로 적었다. 그러나 대부분의 학생들이 한번 이상의 대응 오류를 범하였다. 학습접근 양식에 관계없이 많은 학생들이 비유 만들기에 대해, 개념 이해와 기억 향상, 사고력 증진 등의 인지적 측면과 주의 집중, 친근감, 흥미나 호기심 유발 등의 정의적 측면에서 긍정적으로 인식하는 것으로 나타났다. 반면, 비유 만들기의 어려움, 많은 시간 소요, 대응 과정의 어려움 등과 같은 단점을 지적하기도 하였다.

대한화학회
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열에너지 흡수에 의한 혼합용매의 증발과 온도변화의 관찰 및 이해

이지은, 채윤수, 강은주

송우중학교

중학교 교육과정에서 소개되는 물질의 상태, 상태변화와 에너지, 순물질과 혼합물, 용액의 성질 등을 실험으로 관찰하기 위하여 액체가 기화될 때 주위의 열에너지 변화를 열전대(thermocouple)를 사용하여 온도변화로 측정하였다. 본 연구는 중학생이 실험하였고 실험대상을 관찰하였으며, 그들의 이해정도를 토대로 실험결과를 취합하고 결론을 도출하였다. 물질의 상태변화에 따른 열에너지 변화를 관찰하기 위하여 물, 에탄올, 메탄올, 아세톤, 벤젠 등의 용매와 그들의 혼합용매를 사용하여 기화될 때 열전대 주위의 열에너지 변화를 온도변화로 측정하였다. 준비된 시료에 대한 온도변화의 크기는 각 용매의 분자량, 끓는점, 극성도, 증발열, 및 점도 등으로 비교분석하였고, 혼합용매에서의 온도변화 크기와 비교하여 순물질과 혼합물질 간의 분자간 결합에너지 크기를 비교할 수 있었다. 순물질 액체의 기화는 해당 용매의 물리적 특성에 의존하여 극성이 작고 분자량이 작아 끓는점이 낮은 용매일 수록 증발될 때 가장 큰 온도변화를 관찰할 수 있었다. 혼합용매의 열에너지 흡수에 의한 기화온도변화는 혼합비율과 비례하였으나, 혼합용매의 종류에 따라 정편차 또는 부편차의 결과를 나타내었다.

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CoRe에 기반한 밀도 개념 수업이 개념형성과 수업만족도에 미치는 영향

최병순

한국교원대 화학교육과

이 연구에서는 CoRe 에 기반한 밀도 개념 수업이 개념형성과 수업만족도에 미치는 영향을 알아보기 위하여 중학교 2 학년 6 개 학급 240 명을 대상으로 연구하였다. CoRe 에 기반한 밀도 개념 수업은 기존에 밀도에 관해 연구된 CoRe 를 분석하여 이를 바탕으로 4 차시분으로 구성하였다. 실험집단과 통제집단의 개념형성 정도를 비교하기 위해 밀도 개념 수업 후 사후 검사를 실시하였으며, 수업을 실시한 3 개월 후에 파지 정도를 검사하여 비교하였다. 또한 실험집단에 대해서는 수업만족도 검사를 실시하였으며, 과학관련 태도수준과 학업성취수준을 기준으로 수업만족도를 분석하였다. 연구 결과, 실험집단이 통제집단보다 사후검사와 파지검사에서 모두 유의하게 높게 나타났다. 이는 CoRe 에 기반한 수업이 학습자가 가지고 있는 선개념의 유형과 학습과정에 있어서 학생, 교사, 환경, 평가 등 다양한 영역의 어려움과 한계점을 인식하고, 이를 최대한 해결하고자 하는 수업전략을 중심으로 이루어져 있기 때문이라고 해석된다. CoRe 에 기반한 수업에 대한 만족도를 분석한 결과, 전반적으로 수업만족도가 높게 나타났으며, 특히 과학관련 태도 수준이 높거나, 학업성취 수준이 높은 학생이 높은 수업만족도를 보였다. 인터뷰 결과, 실험 집단은 CoRe 에 기반한 수업을 통해 다양한 생각을 할 기회가 있었던 점, 개념을 제시하는 것이 아닌 찾아가는 방식으로 예측해보고 결과를 확인하는 수업방식, 학생 스스로 수업에 적극적으로 참여하도록 유도한 점 등에 긍정적인 만족도를 보였다.

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과학적 모델의 분류틀 개발 및 모델 예시에 대한 학생과 교사의 이해 분석

장은경, 강성주

한국교원대 화학교육과

이 연구의 목적은 고등학교 화학 교과서에 제시된 여러 모델을 분류하여 화학 교육에서 사용되는 과학적 모델의 분류틀을 개발하고 모델 예시에 대한 학생과 교사의 이해 정도를 분석하고자 하는 것이다. 고등학교 화학Ⅱ 교과서의 과학적 모델을 분석하고 과학적 모델의 분류틀을 개발하여 과학교육 전문가와 동료 연구자의 검증을 받아 수정하였다. 12 가지 모델의 예시에 대한 학생과 교사의 이해 정도를 분석하기 위해 인문계 고등학교 3 학년 자연계열 학생 139 명과 화학 전공의 현직 교사 33 명을 대상으로 설문지 조사를 시행하였다.연구 결과, 고등학교 화학 교육에서 활용되는 과학적 모델의 분류틀은 크게 추상적 모델과 물리적 모델로 나누어질 수 있다. 추상적 모델은 다시 수학적 모델, 비유 모델, 화학식 모델로 세부 분류되며, 물리적 모델은 분자 구조 모델, 입자 모델, 실험적 모델로 세부 분류된다. 모델 예시에 대한 학생과 교사의 이해 유형 분석 결과 학생과 교사 모두 대체로 예시에 대한 모델의 종류를 적절하게 선택하고 있음을 알 수 있었다. 학생과 교사의 정답률은 대체로 높았으며, 특히 교사의 경우 전반적으로 거의 모든 문항에서 정답률이 높았다. 오답을 선택한 응답자는 각 세부 모델별 모델에 대한 정의를 숙지하지 않은 상태에서 예시에 대해 직관적으로 설문에 응답한 경우가 많았다. 모델의 예시에서 플라스크나 비커 등이 표현된 있는 경우 교사와 학생 일부는 실험 기구 자체에 중점을 두고 실험적 모델로 한정 짓는 경우가 나타났으며, 전자가 점으로 표현된 경우에는 교사와 학생 일부가 점으로 표현되었다는 사실 자체에 중점을 두고 입자 모델로 한정 짓는 경우가 나타났다.이러한 연구결과로부터 화학교육에서 사용되는 과학적 모델의 분류틀을 이용하여 실제 수업에서 학생들이 스스로 다양한 모델을 창안하고 표현해보게 하는 시도가 이루어지기를 기대한다. 본 연구에서 사용한 분류틀을 발견법적인 도구로 삼아 화학자들이

사용하는 모델과 모델링 과정을 분석해 볼 필요가 있다. 또한 새롭게 발견되는 모델이 있거나 화학교육에서 사용되는 과학적 모델을 분석할 수 있는 다른 차원의 속성이 발견될 때에는 기존의 분류틀을 수정하는 작업이 이루어져야 할 것이다.

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일반화학의 관점에서 본 고등학교 화학과의 연계성 분석

문숙희, 이상좌

목포대 화학과

고등학생들이 이공계 대학으로 진학하는 경우 고등학교 화학 교과 과정은 대학에서 배우는 일반화학의 기초가 되므로 서로 깊은 연관성을 갖게 된다. 따라서 고등학교에서는 화학 Ⅰ 및 화학 Ⅱ를 배움으로써 화학의 기본 개념을 익혀 개념 체계가 형성되도록 하고 있다. 그러므로 대학 과정과의 연계성 측면에서 고등학교 화학 교육과정의 방향 설정이 매우 중요하다. 본 연구에서는 제 7 차 교육과정에서 사용되고 있는 현 고등학교 화학 Ⅰ 및 화학 Ⅱ의 출판사별 7 종 교과서와 대학에서 사용하고 있는 일반화학 교재의 내용을 비교 분석하여, 연관성을 파악해보았다. 더불어 대학교 1 학년 학생들을 대상으로 한 설문조사 연구를 통해 고등학교와 대학교 일반 화학의 연계정도를 어떻게 파악하고 있는지 분석해 보았다.

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발표종류: 포스터, 발표일시: 금 10:30~12:30

Relationship between Chemistry Lab Notebooks and Academic Achievement for Gifted Science Students

김동진, *백인환, *박국태

*병점고 교무실 *한국교원대 화학교육과*

The purpose of this study was to analyze chemistry laboratory notebooks completed by gifted science students and investigate their observations on chemistry experiments and the laboratory notebooks. The correlations between the students' mid-term academic achievement (MAA) scores and the holistic grading scale (HGS) and lab note rubric (LNR) scores for their chemistry laboratory notebooks were examined. Through an e-mail questionnaire, the gifted science students, now in university, gave their observations of the chemistry experiments and the laboratory notebooks. Based on the correlations between the student's midterm scores and their chemistry experiment laboratory notebook scores, the students were divided into four groups and one student from each group was selected for a semi-structured telephone interview. According to the results of the study, the MAA scores and chemistry LNR scores were more correlated than the MAA scores and chemistry HGS scores. The students were separated into 4 types based on the relationship between their scores and their chemistry LNR scores. They felt they got a better understanding of experimental procedures and data analysis by doing laboratory experiments. Also, they thought that completing the chemistry laboratory notebook in science high school and university was beneficial for gifted science students.

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고등학생들의 성격유형에 따른 관찰 특성 분석

정영은, *박현주, **민병욱

*조선대 과학교육과 *조선대 과학교육학부 **오성고*

21 세기 과학기술지식기반 사회에서 개인과 국가의 경쟁력은 폭주하는 지식과 정보를 어떻게 활용하고 창출하는가에 달려 있다. 창의성은 새로운 아이디어를 산출할 수 있는 능력, 새롭게 산출된 아이디어가 인간과 세계의 관계를 재구성하며 삶의 틀을 확장시킬 수 있는 가능성이다. 관찰은 과학 영역 뿐만 아니라 시, 그림 그리기 등과 같은 창작 활동과 상상력의 기본이 된다. 과학에서의 관찰은 과학적 탐구 과정 기능 중 가장 기초적이며 중요한 것으로, 감각기관을 이용하여 주위 환경으로부터 양적·질적 데이터를 수집하고 기술하는 능력이다.한편, 관찰은 감각 기관에 의해서만 이루어지는 것이 아니라 두뇌의 인지적 과정을 거쳐 이루어지는 것이므로 외부의 동일한 감각정보도 개인에 따라 다르게 인식할 가능성이 매우 크며, 관찰 행위에 의해서 영향을 받을 뿐 아니라 이론에 의해서도 영향을 받는다. 거의 모든 지식의 생성과 창조물은 관찰의 산물이기에, 관찰과 창의성은 사실 불가분의 관계에 있다. 그러나 창의성과 관련된 선행 연구들은 다양한 접근방법을 사용하였으나 창의성 활동에서 가장 중요하고 기본적인 '관찰'을 활용한 접근방법은 시도되지 않았고, 과학교육 분야에서도 관찰은 기본 탐구 능력에 해당하다고 인식되어 왔지만, 학생들이 가지고 있는 관찰의 특성과 행태에 대해서는 제한적으로 연구가 진행되었다. 이 연구는 고등학생들의 성격유형에 따라 주어진 관찰 대상에 대한 관찰의 행태는 어떠한가를 조사하였다. 연구 자료는 고등학생들을 MBTI 를 이용하여 성격유형을 조사하고, 주어진 관찰 대상에 대하여 자유롭게 관찰하도록 함으로써 수집하였다. 그 결과, 성격유형에 따라 관찰 행태가 차이가 있음을 알 수 있었다.

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중학생들의 성격유형과 과학탐구능력의 관계 분석

천희진, *박현주, **민병욱

*조선대 과학교육 *조선대 과학교육학부 **오성고*

과학탐구능력이란 과학자들이 조사하고 연구에 필요한 능력으로, 학생들이 어떤 문제에 부닥쳤을 때 과학적 탐구방법에 의해 스스로 문제를 해결하는 능력이다. 이 과학탐구능력은 범내용(content free)적으로 일상생활에서 높은 전이 효과가 있는 것으로 믿어진다. 과학탐구능력의 향상은 과학적 사실과 과학적 개념을 잘 이해할 수 있고 실험능력을 향상시킬 수 있는 것으로 기대된다. 과학탐구능력에 영향을 주는 변인들에 대한 연구는 꾸준히 진행되어 왔다. 개인에게 효과가 있는 방법을 결정하기 위해 발견된 가장 유용한 도구는 인간의 성격과 관련된 기질 이론과 성격유형 이론이다. 기질과 성격유형 이론에 따르면, 사람들은 서로 다른 존재들이기 때문에 배우고 가르치는 방법도 다르다. 이 연구에서는 과학탐구능력의 관찰, 분류, 측정, 추리, 예상, 자료변환, 자료해석, 가설설정, 변인통제, 일반화 등 이러한 능력들이 개인의 성격 유형과 어떤 관계가 있는지를 조사하였다. 중학생을 연구대상으로 하여, MBTI 와 과학탐구능력검사지를 이용하여 학생들의 성격유형과 과학탐구능력을 조사하였다. 연구결과, E/I 지표는 탐구요소 중 관찰, 추리, 자료해석, 가설설정, 총점이 내향성과 유의미한 상관관계를 가지는 것으로 조사되었다. S/N 지표는 추리와 직관형, T/F 지표는 추리와 사고형, J/P 지표는 측정과 인식형이 유의미한 상관관계가 있는 것으로 나타났다.

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Experimental study on the enhanced CO_2 hydrate stability in Ulleung-basin soil suspension

이경진, 이우진

KAIST 건설및환경공학과

Since the discovery of natural gas hydrate (NGH) reservoir in Ulleung-basin area, East sea of Korea, geological formations of NGH-bearing sites has been considered to provide proper sites for CO_2 storage. We investigated the stability of CO_2 hydrate by measuring its phase equilibrium corresponding to the physical and geochemical conditions of the Ulleung-basin environment. Experimental three-phase (aqueous liquid suspension – vapor CO_2 – incipient hydrate) equilibrium conditions of CO_2 hydrate dissociation in aqueous suspensions of electrolyte (NaCl 3.5%) and marine sediments (10mg/mL) from Ulleung-basin were measured in the temperature range of 270 – 280 K and pressure range of 0.9 – 3.5 MPa. It was observed that equilibrium conditions including Ulleung-basin soil shifted to lower pressure and higher temperature region compared to the pure CO_2 hydrate equilibrium. We investigated the effect of Ulleung-basin inorganic mineral components on the equilibrium conditions by varying the soil mineral types of the suspensions. Quartz and Illite were chosen as the representative soil mineral of Ulleung-basin soil, as based on its quantitative XRD result. We further checked the effect of the organic component on the equilibrium conditions by adding a biosurfactant (20μM) in the system. The experimental results show that particular interactions under different mineral types and presence of a surfactant could lead to different CO_2 hydrate equilibrium conditions. It is implied that Ulleung-basin soil alter the CO_2 hydrate equilibrium conditions due to its inorganic soil mineral components and due to its organic fractions as well.

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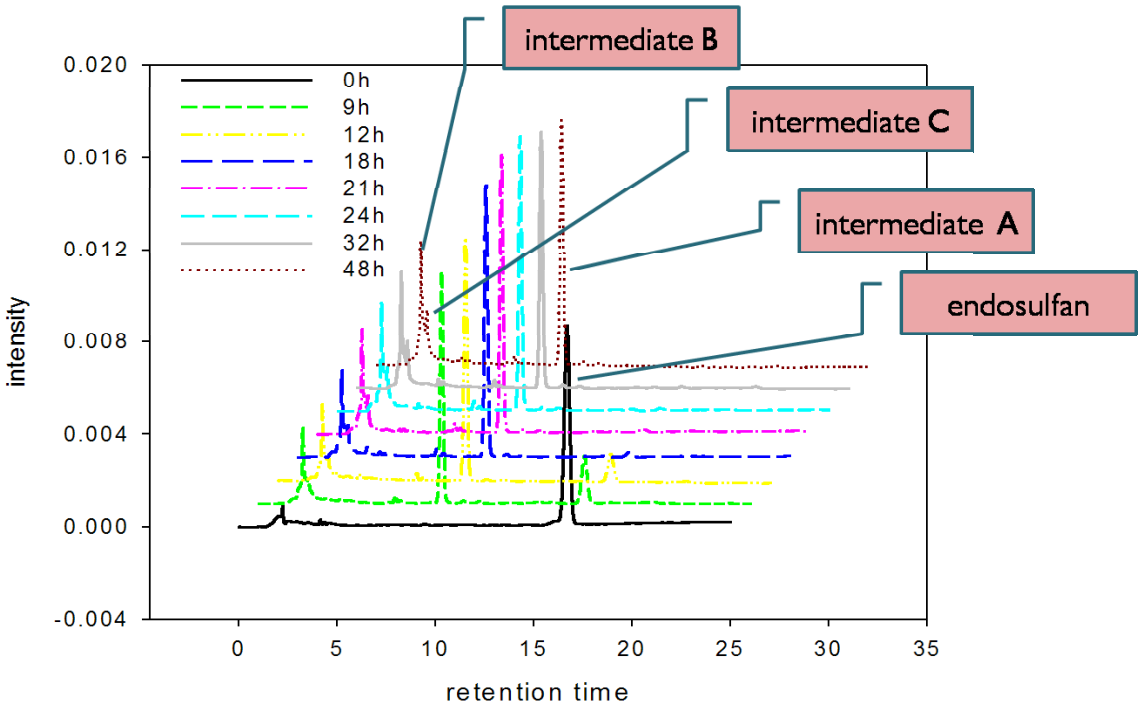
Mechanistic aspects in the degradation of XOCs(halogenated organic compounds) by zerovalent iron

안삼영

순천대 환경교육과

The reductive degradation of XOCs has been carried out by the reaction with zerovalent iron under the oxygen free condition. The properties of zerovalent iron, such as particle size, dosage and manufacturer, the concentration of XOCs, and pH of the solution have an influence on the decomposition reactivity and the reaction process. In this study, we selected an organochlorine pesticide, endosulfan, which is a widely used organochlorine pesticide in korea. The formation of intermediates and thier transformation has been monitored under diverse reaction conditions. In our preliminary experiments, five intermediates were detected in HPLC and their relative intensity changed with time. Their isolation and the structural characterization are under investigation.



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Influence of natural organic matter on enhanced CO2 hydrate formation for its sequestration

Rheo B. Lamorena, 이우진

KAIST 건설및환경공학

A study was conducted to investigate the effect of natural organic matter on CO2 hydrate formation. Marine sediments from a gas hydrate reservoir in Ulleung Basin were used to identify the role of organic matter and its controlling factors for the hydrate formation. 1H-NMR, FTIR, MLOI (10%) and TOC (13-15 ppm) analyses of the sediment samples showed that significant amounts of organic matter exist in the samples. CO2 hydrate formation tests were conducted using the marine sediments at 0.3 0C and 30 bar. Control samples were also prepared with kaolinite suspensions. All marine sediment suspensions showed early hydrate formation (~40 min) compared to that in the control test (>300 min). Extraction procedures were carried out on the marine sediment samples to characterize the extracts which potentially influence the enhanced hydrate formation. Results showed that the extracted humic fraction promotes earlier hydrate formations as compared with non-polar and polar fractions. The experimental results can contribute to our understanding of hydrate formation processes and its feasible application to the CO2 sequestration in natural and engineered deep-sea environments.

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Multi-Dimensional Correlation Analysis on CO_2 Emission and Cost of Energy Resources

김희태, 김은철, 안태규

성균관대 에너지과학과

World moves towards a post-carbon society and needs clean and renewable energy for sustainable development. There are many kinds of methodological approaches which help the shift based on analyzed data about energy resources and which focus on limited types of energy including liquid fossil, solid fossil, gaseous fossil and biomass (eg. *1996 Guidelines* [1], *GPG2000* [2], *GPG-LULUCF* [3], and *2006 Guidelines* [4]). But we should consider the amount of CO2 emission and cost of the renewable energy to make a better decision. In this work, we analyze an economic cost with carbon emission factor to present a correlation between CO_2 emission and cost of energy sources under the same potential energy.

1. *The Revised 1996 IPCC Guidelines for National Greenhouse Gas Inventories*, IPCC, 1997
2. *The Good Practice Guidance and Uncertainty Management in National Greenhouse Gas Inventories*, IPCC, 2000
3. *The Good Practice Guidance for Land Use, Land-use Change and Forestry*, IPCC, 2003
4. *2006 IPCC Guidelines for National Greenhouse Gas Inventories, Prepared by the National Greenhouse Gas Inventories Programme*, IPCC, 2006

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A study on removal of hexavalent chromium in the cement

강채훈, 김영훈, *김종현, **전종원, 권순덕

*안동대 환경공학과 *경북과학대학 화장품계열 **안동대 응용화학과*

6 가크롬의 높은 독성으로 인하여 시멘트에 포함되어 있는 6 가크롬이 연구자들의 관심을 끌고 있다. 국내에 시판되고 있는 시멘트에는 미량의 6 가 크롬이 포함되어있으며 본 연구에서는 환원적 방법에 의해 시멘트에 포함되어 있는 6 가크롬을 제거하고자 하였다. 6 가 크롬을 제거하기 위해 FeSO4, zerovalent iron, magnetite, hematite, iron Chloride 를 이용하여 연구를 하였다. 시멘트 제조사 별로 각각의 FeSO4, zerovalent iron, magnetite, hematite, iron chloride 양을 달리하여 첨가한 후 교반한 상태에서 반응시간을 다양하게 설정하고 원심분리 후 상등액만 추출하였다. 추출한 상등액을 산성조건에서 디페닐카르바지드를 이용하여 적자색의 착화합물을 형성하는 것을 UV 540nm 에서 측정하였다. 측정결과 zerovalent iron 을 사용한 경우에는 시멘트에 있는 6 가 크롬의 초기농도보다 10~50%의 제거된 것을 관찰 할 수 있었고 FeSO4 를 사용한 경우에는 60~80%의 제거율을 볼 수 있었다. 이 중 iron chloride 를 사용한 것에서 70~90%로 가장 제거율이 좋게 나타났다.

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Accelerated Cr(VI) reduction by organic reductants in ice

김기태, 최원용

포항공과대 환경공학부

Chromium redox chemistry is important process not only in nature but also engineering. Hexavalent chromium reduction arrest attention much in the field environmental science because of its acute toxicity. Cr(VI) reduction in the presence of various organic reductants, which takes place very slowly in aqueous solution, was significantly accelerated by freezing. The accelerated Cr(VI) reduction reaction by freezing is explained by enriched organic reductant and lowered pH value in ice crystal grain boundaries, that is “freeze concentration effect” and “pH effect” respectively. The enhanced Cr(VI) reduction by freezing indicates new pathway of natural Cr(VI) reduction process and exhibits environmental friendly treatment of Cr(VI) waste water.

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Visible Light Sensitized Production of Hydrogen Using Tin-Porphyrin/TiO_2: A Case of Non-Adsorbing Sensitizer

김우열, *Changhong Li, *김희준, 최원용

*포항공과대 환경공학부 *금오공과대 응용화학과*

Photochemical production of hydrogen is being intensively investigated as a mean of storing solar energy as a chemical fuel. Dye-sensitized semiconductor oxides (e.g., TiO_2) have been frequently studied for this purpose. The efficient visible light sensitization requires a strong chemical binding between the semiconductor surface and the sensitizer molecule. Many sensitizers such as Ru-complexes, Zn-porphyrins and Pt-complexes have been fixed on the surface of TiO_2 through chemical anchoring groups (e.g., carboxylate). However, such chemical anchoring bond can be made only in a specific pH range and not inherently stable in an aquatic environment. This study reports an efficient tin porphyrin (SnP)-sensitized TiO_2system for hydrogen production under visible light in which the adsorption of the sensitizer on TiO_2 is not needed and the H2 production is active over a wide range of pH 3-11. The apparent photonic efficiency for H_2 evolution in SnP/TiO_2 system was estimated to be 35% at 550 nm. Being less expensive, less toxic, and consisting of a more abundant element unlike the Ru-based sensitizers, SnP can be utilized as a practical sensitizer for solar chemical conversion.

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EDTA-TiO_2 Charge Transfer Complex 의 가시광 활성과 반응 메커니즘 규명

김건우, 최원용

포항공과대 환경공학부

The synthesis of visible light active photocatalysts is of great interest for solar energy utilization. Although the most popular photocatalyst TiO2 has demonstrated successful performances for environmental remediation, its application for solar energy conversion is limited because of its large bandgap energy. Among many methods to modify TiO2 for visible light activity, the formation of charge transfer complexes on the surface of TiO2 has been recently investigated. In this study, we investigated the formation of charge transfer complex between TiO2 and EDTA that can absorb visible light through ligand-to-metal charge transfer (LMCT) mechanism. The surface complex between TiO2 and EDTA absorbs considerable amount of visible light at around 400~500nm and this visible light absorption was drastically reduced when the complex formation was inhibited by the surface fluorination of TiO2. The isoelectric point (IEP) of TiO2 particles suspended in water was gradually shifted to lower values with increasing the concentration of EDTA, which supported the formation of surface complex between TiO2 and EDTA anions. The FT-IR spectra of TiO2-EDTA complex showed a clear peak at the wavenumber of 1409 cm-1 which corresponds to the surface-complexed carboxylate group on TiO2 surface. Although the surface complex formation between TiO2 and EDTA has already been reported, the visible light activity of TiO2-EDTA complex has not been recognized. TiO2-EDTA complex exhibited a marked visible light activity. The TiO2-EDTA photocatalyst could reduce Cr(VI) to Cr(III) and produce H2 from water under visible light. The H2 production rate was optimized when EDTA concentration was 100 μM and rutile TiO2 showed higher efficiency than anatase TiO2 samples.

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Photocatalytic Activities of Platinized WO3: The Role of OH Radicals

김정원, 최원용

포항공과대 환경공학부

In most studies on Pt/WO3 photocatalysis, the only aliphatic compound such as acetaldehyde, acetic acid and isopropyl alcohol was used as target substrates and the only role of valence band holes as reactive oxidizing species was emphasized. However, not only valence band holes but also OH radicals which is generated through two pathways, conduction band electrons mediated reduction of O2 and valence band holes mediated oxidation of OH- (or H2O), can play a significant role for the degradation of specific aquatic pollutants.

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Acidification and Pollution Characteristics of Precipitation in JejuCity during the year of 2009

신승희, 고희정, 강창희, 김원형

제주대 화학과

Total 55 precipitation samples were collected in Jeju City during the year of 2009, and their major ionic components were analyzed. The reliability of analytical data of precipitation has been evaluated by the comparison of ion balance, electric conductivity and acid fraction. In the results, their correlation coefficients were in the range of 0.922～0.998, indicating the good quality of collected data. The volume-weighted mean pH and electric conductivity were 4.6 and 22.7 μS/cm, respectively, with the ionic strength of 0.43±0.58 mM. The major precipitation components showed high concentration by the order of Cl^- > Na^+ > nss-SO_4^{2-} > H^+ > NH_4^+ > NO_3^- > Mg^{2+} > nss-Ca^{2+} > K^+ NO_2^- > PO_4^{3-}. The acidification contribution of nss-SO_4^{2-} and NO_3^- showed 98.1%. Meanwhile, the neutralization ratio by NH_3 and $CaCO_3$ were 56.2% and 36.1%, respectively.

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Analysis of Butyltin Compounds in Crassostrea gigas and Tapes philippinarum on the Korean coast.

이성언, *이용우, *원호식, 이동섭

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Tributyltin (TBT) use has been prohibited by the IMO (International Maritime Organization), as well as Korea, since 2003. This prohibition has effected a gradual reduction of TBT use in maritime environs (seawater, sediment, biosamples) in several countries. In this study, crassostrea gigas (oyster) and tapes philippinarum (manila clam), were chosen and measured for butyltin compound concentration, to verify TBT pollution level since its ban in 2003. Specimens were taken directly from farms, for concentration measurement, where crassostrea gigas or tapes philippinarum are cultivated, as well as prevalent locations predicted to have been polluted. Concentrations of MBT, DBT and TBT of crassostrea gigas were measured to be N.D-N.D., N.D.-N.D. and N.D.-60.21 respectively. As for tapes philippinarum, MBT, DBT and TBT were N.D.-12.27, N.D.-45.95, N.D.-7.30 respectively. For this research, a correlative study was conducted to determine butyltin compound concentration in crassostrea gigas at the locations where measurements were made in 1994 to determine to what extent TBT pollution level decreased. A decrease in all 7 sites was observed. In 4 of these 7 samples, butyltin compounds were measured to be below the detection limit. That of tapes philippinarum did not appear high compared to foreign research data. The ban of TBT in Korea in 2003 was thus confirmed to have decreased TBT concentrations on Crassostrea gigas on coastal Korea.

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Enzymatic colourations driven by homo- or hetero-polymer synthesis

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Laccase efficiently catalyses polymerization of phenolic compounds. However, knowledge on applications of polymers synthesized in this manner remains scarce. Here, the potential of laccase-catalysed polymerization of natural phenols to form products useful in hair dyeing was investigated. All 15 tested phenols yielded coloured products after laccase treatment and colour diversity was attained by using mixtures of two phenolic monomers. After exploring colour differentiation pattern of 120 different reactions with statistical regression analysis, three monomer combinations, namely gallic acid and syringic acid, catechin and catechol, and ferulic acid and syringic acid, giving rise to brown, black, and red materials, respectively, were further characterized because such colours are commercially important for grey hair dyeing. Selected polymers could strongly absorb visible light and their hydrodynamic sizes ranged from 100 to 400 nm. Analyses of enzyme kinetic constants,liquid chromatography and electrospray ionization-mass spectrometry (ESI-MS) coupled withcollision-induced dissociation MS/MS indicate that both monomers in reactions involving catechin and catechol, and ferulic acid and syringic acid, are coloured by heteropolymer synthesis, but thegallic acid/syringic acid combination is based on homopolymer mixture formation. Comparison ofcolour parameters from these three reactions with those of corresponding artificial homopolymer mixtures also supported the idea that laccase may catalyse either hetero- or homo-polymer synthesis. We finally used selected materials to dye grey hair. Each material coloured hair appropriately and the dyeing showed excellent resistance to conventional shampooing.Our study indicates that laccase-catalysed polymerization of natural phenols is applicable to thedevelopment of new cosmetic pigments.

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Application of grape seed and its natural polyphenol extracts as a natural organic coagulant in dye-contaminated wastewater

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Natural organic coagulants (NOCs) such as chitosan and Moringa oleifera seeds have been extensively characterized for potential application in water treatment as an alternative to metal-based coagulants. However, the action of both chitosan and M. oleifera seeds is mainly restricted to anionic organic pollutants because of their cationic functional groups affording poor cationic pollutant coagulation by electrostatic repulsion. In this study, we employed ethanolic grape seed extract (GSE) and grape seed-derived polyphenols such as tannic acid and catechin in an effort to find novel NOCs showing stable anionic forms for removal of cationic organic pollutants. The target substances tested were malachite green (MG) and crystal violet (CV), both mutagenic cationic dyes. Polyphenol treatment induced fast decolorization followed by gradual floc formation concomitant with red or blue shifts in maximum absorbance wavelengths of the cationic dyes. Liquid chromatography analysis of flocs formed by polyphenols directly showed that initial supramolecular complexes attributed mainly to electrostatic attraction between polyphenol hydroxyphenyl groups and cationic dyes further progressed into stronger aggregates, leading to precipitation of dye–polyphenol complexes. Consistent with the results obtained using catechin and tannic acid, use of GSE also resulted in effective decolorization and coagulation of soluble MG and CV in aqueous solutions. Screening of several organic GSE components for NOC activity strongly suggested that natural polyphenols are the main organic ingredients causing MG and CV removal via gradual floc formation.The treatment by natural polyphenols and GSE decreased toxicity of MG- or CV-contaminated water.

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철 환원 미생물에 의해 생성된 2가 철에 의한 1,1,1-TCA 및 PCE 의 분해 연구

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철 환원 박테리아 (Geobacter, Shewanella..etc)의 환원능에 대한 연구는 magnetite, goethite, hematite, lepidocrocite 그리고 nontronite 등, 여러 종류의 Fe3+ 함유 광물의 환원에 대해서 집중적으로 연구되어져 왔다. 이렇게 철 환원 박테리아에 의해 Fe3+가 Fe2+ 로 환원된 Fe2+는 화학적 탈 염화과정에 필수요소인 Fe2+를 증가시켜주어 유기 염소계 화합물의 분해 반응을 촉진시킬 수 있다고 알려진다. 이번 연구에서는 철 환원 박테리아로 Shewanella putrefaciens CN32 , Fe3+ 함유 광물로는 magnetite, lepidocrocite, hematite 그리고 nontronite 를 이용하여, 대표적인 유기 염소계 화합물인 1,1,1-TCA 와 PCE 분해에 대한 kinetic test 를 하였다. 기존의 박테리아를 접종시키지 않은 샘플에서는 시간에 따른 0.5 N HCl 에 추출 가능한 Fe2+ 농도가 증가 하지 않는 반해, 박테리아를 접종 시킨 샘플인 경우에는 모든 철함유 광물에서 Fe2+ 농도가 2 달 동안 현저히 증가 한 것을 관찰 할 수 있었다. Fe3+ 환원속도를 비교한 결과 magnetite > lepidocrocite > nontronite > geothite = hematite 순서로 나타났으며, SEM 이미지를 결과를 보면 위와 같은 순서로 각 미네랄 표면에 박테리아의 안착이 잘 보이는 것으로 나타났다. 1,1,1-TCA 와 PCE 에 대한 magnetite 의 분해능을 살펴본 결과, 기존의 magnetite suspension 에서는 별다른 분해를 보이지 않은 것 과 대조해서 Shewanella 를 접종한 magnetite suspension 에서는 약 75% 의 1,1,1-TCA 와 20% 의 PCE 가 분해 되었다는 것을 관찰 할 수 있었다.

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새로운 철이온 안정화 물질(cross-linked chitosan)을 이용한 개선된 펜톤 반응에서의 사염화탄소 분해 메커니즘 연구

신영호, *이영민, **이우진

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염소계 화합물은 다양한 산업 분야에서 사용되고나, 사용자 부주의 및 노후 시설로 인해 자연계에 노출될 경우 그 독성과 난분해성으로 인해 치명적인 악영향을 미칠 수 있다. 이러한 염소계 화합물로 오염된 토양 및 지하수 복원을 위한 방법으로는 생물학적, 그리고 물리/화학적 방법들이 있다. 이중 펜톤 기술은 철이온과 과산화수소를 이용하여 강력한 산화제인 수산화 라디칼을 형성하는 기술로써 대부분의 유기화합물을 빠른 시간 내에 분해할 수 있으며, 환경친화적인 이유로 인해 실제 오염부지에 많이 적용되었으며 현재에도 연구 및 개발되고 있는 기술이다. 그러나 염소계 화합물 중 사염화탄소는 위와 같은 전통적 방식의 펜톤반응으로는 제거 효율이 매우 낮은 것으로 알려져 있다. 그 이유는 사염화탄소는 수산화 라디칼에 의한 산화적 탈염소 반응으로는 제거되지 않기 때문이다. 따라서 본 연구에서는 철이온을 안정화시킬 수 있는 새로운 킬레이트 물질인 키토산을 이용한 개선된 펜톤 반응을 통한 사염화탄소의 환원적 탈염소 반응에 대한 연구를 수행하였다.pH 6 에서 키토산에 의해 안정화된 철이온을 사염화탄소 분해에 적용할 경우 펜톤 분해 효율을 크게 향상시킬 수 있었다. 개선된 펜톤반응 내에서 사염화탄소의 분해는 염소이온 농도와 중간 반응산물들을 분석함으로써 탈염소 반응을 통해 일어난다는 것을 증명하였다. 이때, 측정된 모든 시료의 염소이온 회수율은 초기 사염화탄소 농도와 비교하여 91% 이상을 보였다. 또한, 수산화 라디칼의 scavenger 로 잘 알려진 2-propanol 을 이용하여 사염화탄소의 분해가 산화적 분해 반응이 아닌 환원적 분해 반응을 통해 일어남을 보였다. 분해 효율 영향인자로써 과산화수소, 철이온 그리고 사염화탄소 농도를 변화하며 분해 실험을 수행하였다. 추가적인 분해 메커니즘을 증명하기 위한 실험으로 SEM-EDX, TEM 분석을 통해 키토산 표면에 적절히 흡착된 철이온과 XPS 분석을 통해 개선된 펜톤 반응의

개시를 알 수 있었다. 따라서, 키토산을 활용하면 다양한 물질로 오염된 토양 및 지하수의 효과적인 복원이 가능하며, 이는 폐각 자원 활용 측면에서도 환경 친화적인 대체 복원 기술로써 평가 받을 수 있을 것이라 기대된다.

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Pyrite 현탁 시스템 내의 펜톤 산화 반응을 이용한 carbon tetrachloride 제거

채형수, 이우진

KAIST 건설 및 환경공학과

철 함유 토양광물을 이용한 현탁 배치 시스템에서 펜톤 산화를 통한 carbon tetrachloride (CT) 분해 연구를 수행하였다. 다양한 철 함유 토양광물 중 펜톤 산화에서 가장 큰 반응성을 갖는 pyrite 이 과산화수소로부터 산화제를 생성하는 촉매제로 사용되었다. 모든 실험은 pH 3 의 산성조건에서 수행되었으며, 0.43~8.55 g/L pyrite, 54~326 mM 과산화수소가 본 시스템에 적용되었다. Pyrite 의 농도가 높아짐에 따라 CT 제거 반응 상수는 증가하는 것을 볼 수 있고, 이는 pyrite 의 농도가 반응상수에 영향을 미친다는 것을 알 수 있다. 충분한 양의 과산화수소를 시스템에 공급할 경우, CT 제거 반응은 pseudo-first order law 를 따르는 것을 알 수 있다. 반면 과산화수소의 양이 시스템 내의 CT 제거에 충분하지 않을 경우, CT 제거 반응은 과산화수소가 소모됨에 따라 second order law 를 따르는 것을 알 수 있다. OH 라디칼의 방해물질인 2-propanol 을 CT 제거 시스템에 주입했을 때, CT 제거 반응은 보다 촉진되는 것을 알 수 있다. 이는 CT 제거반응은 일반적인 펜톤 반응 경로인 OH 라디칼에 의한 산화적 제거 반응이 아닌 환원적 제거반응임을 알 수 있다. Pyrite 을 이용한 펜톤 반응은 조기 종결되는 기존의 펜톤 반응을 극복하고, 다양한 염소계 화합물을 산화・환원의 복합적인 처리가 가능하기 때문에 폐수 및 지하수 내의 오염물질 제거에 적용될 수 있는 유망한 공정으로 판단된다.

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A study on zeta potential analysis of pyrite suspension in the presence of cationic surfactant at pH 7

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A study was conducted to investigate how the zeta potential of pyrite suspension changes with a range of surfactant concentrations. In this research, 4 g/l pyrite suspension has been equilibrated with 0.1 mM ~ 1.8 mM of cationic cetylpyridinium chloride (CPC) surfactant. The pH of pyrite suspension has been fixed at 7 using 0.1M 3-(N-morpholino) propanesulfonic acid (MOPS) buffer and NaOH. From the zeta potential analysis, it has been observed that the concentration of surfactant could dramatically change the zeta potential of pyrite suspension. At low surfactant concentrations (upto 0.2 mM), the zeta potential value reached from maximum negative value (-5.28 mV) to maximum positive value (36.5 mV) giving the isoelectric point (iep) at 0.12 mM surfactant concentration. With the increasing value of surfactant concentration, the zeta potential started to decrease and from 0.6 mM of surfactant concentration, it gave constant value. The experimental results can contribute to explain the adsorption mechanism of a cationic surfactant on pyrite surface at certain pH condition and this could be applied for the selection of optimum surfactant concentration for maximum adsorption to remove surfactant from selected stages of the industrial process or wastewater emission systems.

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A Novel Synthesis of Nanoscale Iron Particles Using Natural Polyphenols for Enhanced Chromate Removal from Water

장윤석, 김재환

포항공과대 환경공학부

The use of nanoscale zerovalent iron (nZVI) particles to immobilize heavy metals found in contaminated groundwater is a promising technology for in-situ remediation. The ability of nZVI to adsorb and subsequently reduce toxic heavy metals can be enhanced by using stabilizer compounds during nZVI synthesis procedure. Although to date several stabilizers leading to the enhanced ability of nZVI to removal heavy metals have been reported, the stabilizers are expensive and environmental safety is also not guaranteed. Here we for the first time demonstrated that natural extracts obtained from grape skins and seeds that are edible, eco-friendly, cheap, and renewable plant materials can act as efficient nZVI stabilizers for hexavalent chromium (Cr(VI)) removal from water. It was revealed that natural polyphenols that efficiently chelate ferric ions are a main contributor of the nZVI stabilization by evaluating the ability of several organic components of the extracts to induce the enhanced Cr(VI) removal. Further characterization of natural polyphenol-induced nZVI stabilization was performed with tannic acid and gallic acid as a model polyphenol compound. A possible mechanism for the chemical interactions between polyphenol-nZVI and Cr(VI) was proposed via sedimentation, X-ray diffraction, transmission electron microscopy, inductively coupled plasma experiments.

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Kinetics study of Nanoscale Iron Particles Synthesized with Dithionite for Dechlorination of Trichloroethylene

장윤석, 김재환

포항공과대 환경공학부

Extensive studies for synthesis and characterization of novel nanoparticles with unique reactivity and functions have been made during the recent years. Among the nanoparticles, nanoscale zerovalent iron (nZVI) has been used for clinical diagnosis and treatment, as magnetic ferrofluids, in catalysis and as environmental remediants. The remediation of groundwater contaminated caused by chlorinated organic compounds (PCE, TCE) is a demanding issue worldwide. These compounds are frequently found in groundwater of industrial complex, land fill site, and leaking tanks. To remove these chlorinated compounds, reliable cost-effective methods are needed, iron has been used to treat chlorinated organic compounds. In this study, we show that nano-sized zero valent iron (nZVI) and D/nZVI which was synthesized with dithionite dechlorinate trichloroethylene (TCE) effectively. The addition of dithionite might reduce the amorphous iron oxide on the surface and make a magnetite phase. The rate of TCE dechlorination using D/nZVI (synthesized with dithionite) was 4 – 8 times of magnitude faster than typical nZVI. The magnetite probably might to increase the reaction rate for trichloroethylene, result in rapid dechlorination. Each reaction rate constant was discussed in here.

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