일시: 2014년 4월 16~18일(수~금) 3일간

장소: 일산KINTEX

발표코드: **PLEN-1**

발표분야: 기조강연

발표종류: 특별강연, 발표일시: 목 16:30, 좌장: 신승구

Plasmon-molecule interactions

George C. Schatz

Northwestern University, USA

This talk describes recent theory developments concerned with the optical properties of plasmonic materials, with emphasis on understanding plasmon enhanced spectroscopic techniques such as SERS, plasmon-enhanced photochemistry, and the coupling of plasmons to excitons. The cornerstone of this work is computational electromagnetics, which provides the ability to solve Maxwell’s equations exactly for a given nanoparticle structure and with assumed dielectric functions. A number of methods for doing these calculations are available, and in the first part of the talk we show how one can use them to study important problems of interest in plasmonics. These applications show how small gaps (1 nm) between 100 nm silver or gold nanoparticles lead to electromagnetic hot spots with multipole plasmon modes that produce the largest SERS enhancements when dark plasmon modes are excited, in part due to excitation of the dark modes by Raman emission. This application shows that classical electrodynamics needs to be coupled to quantum mechanics for a quantitative description of SERS, so the second half of the talk will focus on methods that couple electrodynamics calculations with TDDFT either in real-time or with frequency domain calculations. Inclusion of both electromagnetic interactions and chemical interactions between the metal nanoparticle and molecular adsorbate are considered. We demonstrate the use of these QM/ED methods with applications to SERS and to plasmonic solar cells. In addition, we describe several examples of plasmon-exciton interactions, such as occurs in plasmon-enhanced lasing. Here we show how plasmons can interact with molecules to enhance both spontaneous and stimulated emission.

일시: 2014년 4월 16~18일(수~금) 3일간
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발표코드: **AWARD-1**
발표분야: 기념강연
발표종류: 기념강연, 발표일시: 금 09:00, 좌장: 김종원

Electrochemistry; Bedrock of energy conversion, eco-information processing and biointerface

정택동

서울대학교 화학부

In this talk, we address a few issues that my group has been working on. It starts with electrokinetic examination of intermediate stabilization employing carefully designed redox-active macrocyclic ionophores. A properly functionalized molecule, calix[4]quione, can sequester calcium ion that stabilizes radical anion, intermediate of quinone reduction in aqueous phase, indicating new aspect of molecular switch. Interestingly, electrochemical behavior of quinone near calcium ion captured in an ionophore is very similar to that in nanopores. This is a new route to futuristic electrocatalysis getting over the saga of platinum. In developing better energy storage/conversion devices and sensors, what we need is knowledge about what is happening on the electrode. Unfortunately, there have been only a few ways to make it happen. A great deal of efforts have been made to use surface enhanced Raman scattering (SERS) for this purpose by enhancing the light scattering intensity. In this context, it is truely important to do that regardless of the substrates, which are the electrodes in electrochemistry. We suggested thin gold shells covering micro polymeric beads, which work pretty well as external hot spot assembly and even an ultramicroelectrode(UME) for scanning electrochemical Raman microscopy (SERM). With better understanding electrode kinetics by aid of novel analytical tools, electrochemistry would be able to contribute to numerous technologies that play pivoting roles in industries. Electrodeposition is one of them. We recently came up with exciting concept that enables direct electrodeposition on silicon oxide, well-known dielectric material. Thermally grown silica is a good proton-selective and electrical insulator. We found that the protons permeating through them can serve as electron carriers that allow a pathway of electron flow other than tunneling current. With broad range of audience, I will introduce these thems briefly and discuss widely.

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장소: 일산KINTEX

발표코드: **POLY1-1**

발표분야: Current Trends in Biomedical Polymers

발표종류: 심포지엄, 발표일시: 목 09:00, 좌장: 김원종

The Role of Tauroursodeoxycholic Acid on Adipogenesis of Stem Cells by Modulation of ER Stress followed by Bone Tissue Regeneration

이수홍

차의과학대학교 의생명과학과

Stem cell therapy has been developing rapidly as a potential cure for repairing or regenerating the functions of diseased organs and tissues. For successful therapy, it is required to induce efficient differentiation toward target cells. To date, however, stem cells derived from individual donors not only show wide variations in differentiation potential, also the unclear regulatory mechanisms. The chemical chaperone tauroursodeoxycholic acid (TUDCA) has been known to not only decreases endoplasmic reticulum (ER) stress, but also plays a role as a leptin-sensitizing agent for preadipocytes in mice and humans. In this study, we examine whether TUDCA has an effect on adipogenesis from stem cells followed by bone regeneration. It was found that TUDCA treatment of stem cells significantly decreased in vivo adipogenic tissue formation and enhanced bone regeneration comparing with PBS treatment of stem cells. The results indicate that TUDCA plays a critical role in adipogenesis from stem cells by modulating ER stress as well as bone regeneration, therefore, has potential pharmacologic and therapeutic applications as an anti-obesity agent and bone tissue regeneration, respectively.

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발표코드: **POLY1-2**
발표분야: Current Trends in Biomedical Polymers
발표종류: 심포지엄, 발표일시: 목 09:25, 좌장: 김원종

Robust Optical Nanobiosensors Towards High-throughput Assay

민달희

서울대학교 화학과

Development of practically useful biosensors based on new nanomaterials necessitates understanding and full utilization of chemical/physical properties to detect molecular changes during certain biochemical transformations in a biological system. New system should overcome limitations of conventional assay methods?detection limits, cost issues, labors, efficiencies, quantitativeness, reproducibility, etc. In this talk, I will introduce recent studies which harness graphene derivatives for developing bioanalytical platforms to quantitatively analyze various enzyme activities and biomarkers including helicase and microRNA. The systems rely on attractive interaction between graphene oxide and nucleic acids and fluorescence quenching by graphene oxide. Quantitative microRNA sensing was successfully demonstrated in living cells. Recently, we employed one of the graphene-based bioassay systems to anti-viral drug screening and identified potent hit compounds to treat hepatitis C. This study clearly shows that a new nanobio-technology can be routinely implemented in drug discovery with high-throughput capability, providing many advantages over conventional methods.

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발표코드: **POLY1-3**
발표분야: Current Trends in Biomedical Polymers
발표종류: 심포지엄, 발표일시: 목 09:50, 좌장: 김원종

Thermogelling Polypeptide As a 3D Scaffold for Stem Cell Culture

문효정 고두영 SHINDE USHA PRAMOD 정병문*

이화여자대학교 화학나노과학과

A thermogelling polymer aqueous solution undergoes solution sol-to-gel transition as the temperature increases. We have recently developed a series of thermogelling biodegradable polypeptides, where the secondary structure and nanoassembly play an important role in affecting the material properties. By varying the stereochemistry of amino acids in polypeptides, the molecular weight of hydrophobic/hydrophilic blocks, composition of polypeptides, hydrophobic end-capping of the polypeptides, and microsequences of a block copolymer, thermosensitivity and nanoassembly pattern of the polymers could be controlled. The sol-gel transition mechanism involved changes in secondary structures of the hydrophobic polypeptide and conformation of the hydrophilic block. The polypeptide copolymers were stable in the phosphate buffered saline, whereas their degradation was accelerated in the presence of proteolytic enzymes such as elastase, cathepsin B, cathepsin C, and matrix metallopreoteinase. The thermogelling polypeptide copolymers not only acted as a promising sustained release system for protein drugs but also provided a compatible microenvironment for cells or stem cells, where the cells produced specific biomarkers.

In this presentation, we will discuss our recent progress on cell and stem cell culture by using the polypeptide thermogels.

References

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일시: 2014년 4월 16~18일(수~금) 3일간
장소: 일산KINTEX
발표코드: **POLY1-4**
발표분야: Current Trends in Biomedical Polymers
발표종류: 심포지엄, 발표일시: 목 10:35, 좌장: 박한수

Pluronic-based Nanoparticles for Targeted Cancer Therapy

육순홍

고려대학교 세종캠퍼스 약학과

Pluronic-based nanoparticles were prepared in a melted mixture through temperature-induced phase transition. Polyethylene glycol (Molecular weight: 400) and soybean/Tween 80 mixture were used as solubilizers for paclitaxel (PTX) and docetaxel (DTX), respectively. PTX and DTX, used as model anticancer drugs in this study, are cytotoxic agents belonging to the taxoid family and they have emerged as one of the most important anticancer drugs with proven clinical efficacy against many cancers. The polymer for encapsulation of PTX or DTX was Pluronics (poly (ethylene oxide)-poly (propylene oxide)-poly (ethylene oxide) triblock copolymer, F-68). To examine the morphology and size distribution of Pluronic-based nanoparticles, transmittance electron microscopy and dynamic light scattering were used. The in vitro release behavior, cellular uptake and toxicity were also observed to verify the functionality of Pluronic-based nanoparticles as nanocarriers for anticancer drugs. We verified that temperature-induced phase transitions in a polymer melt formed drug-loaded Pluronic-based nanoparticles for the efficient chemotherapy in fast, simple, solvent-free process. Because of polyethylene oxide group in Pluronic, the long half-life of drug-loaded Pluronic-based nanoparticles in the blood and tumor tissue was accomplished with enhanced therapeutic efficacy above surfactant-based PTX and DTX.

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발표코드: **POLY1-5**
발표분야: Current Trends in Biomedical Polymers
발표종류: 심포지엄, 발표일시: 목 11:00, 좌장: 박한수

Bioinspired and Adaptable Materials from Self-Assembling Biopolymers

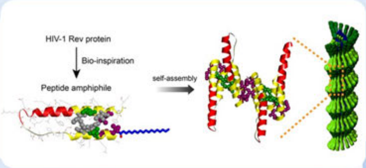
임용범

연세대학교 신소재공학과

In recent years, an interest in manmade or artificial bionanostructures, including peptide-based self-assembled nanostructures has been intense and is expected to escalate further. Proteins are perhaps one of the most diverse and complex structures in nature. Importantly, most natural bionanomachineries are composed of protein. Proteins, similarly to synthetic polymers, are in fact polymeric molecules. Proteins, however, have several unique features when compared to synthetic polymers. One of the most salient features of proteins is that each proteins form unique three dimensional structures, which is determined by their amino acid sequences. When compared to synthetic polymers, another important characteristics of proteins is the monodispersity in molecular weight. When appropriately designed, self-assembling peptide nanostructures can mimic the molecular recognition functions of natural proteins. This research group intends to develop artificial bionanostructures that can mimic or even have enhanced functional properties over the protein-based bionanostructures of biological origin. Moreover, we expect that artificial bionanostructures can be designed to have properties that are unprecedented in nature. Since the major driving force that underlies the formation of bionanostructures is a noncovalent self-assembly process, elaborately designed synthetic self-assembly building blocks should be one of the most suitable candidates for the construction of artificial bionanostructures. In this talk, our recent research efforts towards the understanding of peptide self-assembly process and the development of self-assembled peptide nanostructures as biomedical materials will be presented.

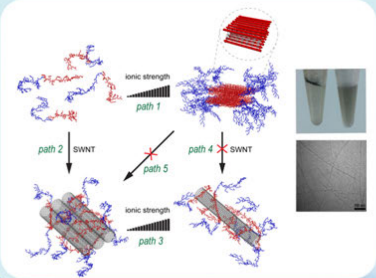
< Bio-inspired Materials >

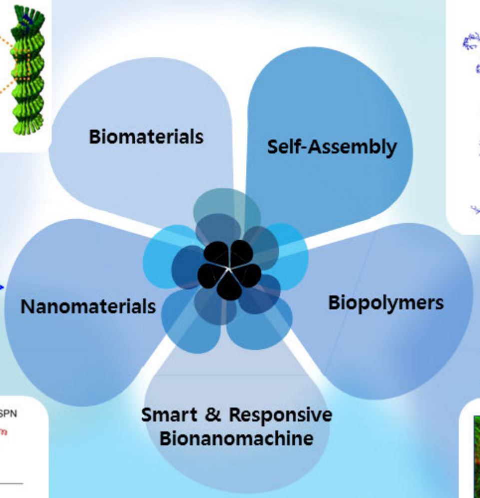
- Development of materials with inspiration from biological nanostructures
- Self-assembling Smart & Responsive Materials



< Biomolecule-Materials Interface >

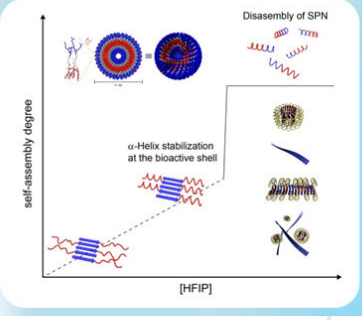
- Controlled self-assembly between biomolecule and nanomaterials for biohybrids development
- Creation of novel and highly functional materials





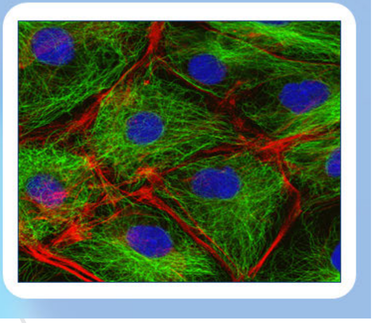
< Self-Assembled Artificial Proteins>

- Construction of functional artificial proteins using simpler peptide building blocks and cost-effective self-assembly process
- Self-Assembly Mechanism & Dynamics



< Therapeutic Nanomaterials >

- Nanomaterials for the modulation of cellular signal transduction network
- Cell function control and disease treatment



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발표코드: **POLY1-6**
발표분야: Current Trends in Biomedical Polymers
발표종류: 심포지엄, 발표일시: 목 11:25, 좌장: 박한수

Photostable Single-Molecule Probes

양시경

전남대학교 화학교육과

Fluorophores, especially those that are bright, photostable, water-soluble, and biocompatible, are powerful tools for studying biological processes in vivo and in vitro. We designed and synthesized a series of perylenediimides (PDIs) encapsulated in polyglycerol dendrons which confer high water-solubility on the PDIs while retaining their excellent fluorescent properties in aqueous media. We have also developed a new, monovalent probe that emits in the far-red region of the visible spectrum with properties desirable for single-molecule optical imaging. This probe is based on a ring-fused boron-dipyrromethene (BODIPY) core that is conjugated to a polyglycerol dendrimer (PGD), making the hydrophobic fluorophore water-soluble. This probe exhibits excellent brightness with an emission maximum of 705 nm. We have observed strikingly long and stable emission from individual PGD?BODIPY probes, even in the absence of anti-fading agents such as Trolox, a combined oxidizing?reducing agent often used in single-molecule studies for improving the photostability of common imaging probes. These interesting properties greatly simplify use of the fluorophore and overcome a significant obstacle in single-molecule fluorescence imaging.

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발표코드: **POLY1-1**

발표분야: Polymeric Materials for Information Technology & Electronics

발표종류: 심포지엄, 발표일시: 목 13:30, 좌장: 김충익

Hole transport and host materials for blue phosphorescent organic light-emitting diodes

이준엽

단국대학교 고분자공학과

고효율 청색 유기발광소자를 개발하기 위해서는 높은 삼중항 에너지를 갖는 유기 물질의 개발이 필요하며 특히 높은 삼중항 에너지를 갖는 정공수송층 물질 및 호스트 물질의 개발이 필요하다. 높은 삼중항 에너지를 구현하기 위해서는 공액 구조가 제한된 방향족 단위들을 도입하는 것이 요구되며, 이를 위해서는 공액 길이가 짧은 다양한 코어 구조를 설계하고 이를 이용하여 유기 재료를 합성하는 것이 요구된다. 본 연구실에서는 최근 다양한 코어 구조를 활용하여 높은 삼중항 에너지를 갖는 화합물들을 개발하였으며, 신규 화합물을 이용하여 30% 이상의 높은 양자 효율을 구현하였다. 본 발표에서는 본 연구실에서 수행한 다양한 구조의 정공수송층 물질 및 호스트 물질에 대하여 소개하고 향후 개발 방향에 대하여 논의한다.

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발표코드: **POLY1-2**
발표분야: Polymeric Materials for Information Technology & Electronics
발표종류: 심포지엄, 발표일시: 목 14:00, 좌장: 김충익

Extrinsic and Intrinsic Charge Transport Property of Organic Semiconducting Polymers

최동훈[*] 조민주 엄현아 이대희 양다슬 신지철

고려대학교 화학과

We can investigate extrinsic charge transport property by using thin film transistors. In addition, the single-crystalline objects will lead us to investigate the intrinsic charge transporting properties of organic semiconducting materials. In the case of crystalline semiconducting polymers, 1-dimensional(1-D) nanostructured objects are fabricated via proper methods such as membrane wetting method and self-assembly in a dilute solution. The aspect ratio of nanowire was modulated with the fabrication method. The internal morphology of elaborated nanowires was investigated by grazing incidence X-ray diffraction and transmission electron microscopy in detail. For instance, transmission electron microscopy and selected area electron diffraction analyses of polymer nanowires made from diketopyrrolopyrrole(DPP)-based copolymer reveal its single-crystalline nature. Highly salient is the fact that the polymer chain axis within the single crystals is parallel to the longitudinal axis of the wire, and the π-π stacking direction is perpendicular to the wire growth direction. High-performance DPP-containing polymers were employed to fabricate the nanowire-based FETs to investigate the intrinsic charge transport property of the polymer, which was compared with those in thin film transistors.

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발표분야: Polymeric Materials for Information Technology & Electronics
발표종류: 심포지엄, 발표일시: 목 14:40, 좌장: 김충익

Field-effect electron transport properties of new polymer semiconductors

KIMFELIXSUNJOO

중앙대학교 화학신소재공학부

Plastic electronics has been expected to realize a novel electronics environment with ubiquitous flexible devices. However, realization of plastic electronics has been delayed due to the scarcity of reliable electron-transporting materials. In this talk, my recent work on high-mobility n-type polymer semiconductors for organic field-effect transistors is presented. We have studied a series of alternating copolymer semiconductors with electron-donating and electron-accepting groups in detail to understand their structure-property relationship. With structural optimization, we have obtained an electron mobility of 0.3 cm2/Vs from a transistor with simple bottom-gate geometry, and demonstrated high-performance complementary circuits based on one of the new polymer semiconductors.

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장소: 일산KINTEX
발표코드: **POLY1-4**
발표분야: Polymeric Materials for Information Technology & Electronics
발표종류: 심포지엄, 발표일시: 목 15:10, 좌장: 김충익

Organic- Inorganic Hybrid Dielectric Materials for Unconventional Electronics

하영근

경기대학교 화학과

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

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장소: 일산KINTEX

발표코드: **POLY1-5**

발표분야: Polymeric Materials for Information Technology & Electronics

발표종류: 심포지엄, 발표일시: 목 15:40, 좌장: 김충익

Sensitive, dynamic and wavelength-tunable photodetectors

정대성

중앙대학교 화학신소재공학부

One of the major drawbacks of conventional Si photodiodes is that they do not have color selectivity and therefore R/G/B color filters must be inserted, which limits the integrity of the pixels. Organic semiconductors and quantum dots have absorption ranges that can easily be tuned by chemical modification and so are attractive candidates for these applications because they can be stacked in a tandem diode that can sequentially detect R/G/B with a much smaller pixel size. Here I review recent progress in solution-processed photodetectors and their applications in everyday and high-end applications, including my own works. Methodologies to build up solution processed photodetectors with high photoconductive gain-bandwidth product are highlighted, together with physical origins behind those results.

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발표코드: **INOR1-1**
발표분야: Past, Present and Future of Inorganic Chemistry in Korea
발표종류: 심포지엄, 발표일시: 목 09:00, 좌장: 나명수

A Pioneer Role in Inorganic Chemistry: The research history of professor Myunghyun Paik’s Group

곽지훈

순천대학교 화학교육과

The research history of professor Paik’s group, ever since the early 1980s, will be introduced. From the early days of the group till the middle of 1990s, metal-promoted reaction was main field of the research. Preparations and reactions accompanying electron-transfer, oxidation and reduction, and template synthesis using transition metal ions were carried out in this period. Especially, a lot of fruitful results were obtained from the template synthesis.Unreachable without transition metal ions and very interesting structure of polyazamacrocycles, having caged rings or functional side chains, with four coordinated or five coordinated macrocycles, etc. were reported. Also, the isolation and study of the catalytic activities of macrocyclic complexes with abnormal oxidation state, monovalent or trivalent, of nickel ions, were a distinctive work. Research field of the group has been expanded dramatically from the late of 1990s, from solution chemistry to solid chemistry, from molecules to supramolecules. Starting from the design and preparation porous coordination networks (PCNs), it has been expanded to the preparation and application of porous metal-organic frameworks (MOFs). The research has been focusing on the development of energy and environment related materials. From these PCNs and MOFs, many fantastic and noble results relating hydrogen storage, carbon monoxide capture, and photo-catalyzed hydrogen generation have been reported until now. Also, molecular dynamics occurring in the crystals of porous frameworks in response to external stimuli has been attracted much attention from a lot of chemists. Conclusively, this group has played a role of pioneer in developing the inorganic chemistry with continually suggesting the hot issue of modern inorganic chemistry.

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장소: 일산KINTEX

발표코드: **INOR1-2**

발표분야: Past, Present and Future of Inorganic Chemistry in Korea

발표종류: 심포지엄, 발표일시: 목 09:20, 좌장: 나명수

Hollow Toroids

김기문

포항공과대학교 화학과

Despite the remarkable progress made in the construction of nano? and microscale architectures with well?defined sizes and shapes by self?assembly, a self?organization?based synthesis of hollow toroids has so far proved to be elusive. Here, we report the first such synthesis using rectangular, flat and rigid core monomers with anisotropically predisposed alkene groups which are cross?linked with each other by dithiol linkers using thiol?ene photopolymerization to create the hollow toroids. The resulting superstructures are shape?persistent and mechanically robust in solution. In addition, their size can be tuned by controlling the initial monomer concentrations, an observation which is supported by a theoretical analysis. These hollow microrings can encapsulate guest molecules in the intratoroidal nanospace and act as templates for circular arrays of metal nanoparticles on their peripheries.

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발표코드: **INOR1-3**
발표분야: Past, Present and Future of Inorganic Chemistry in Korea
발표종류: 심포지엄, 발표일시: 목 09:40, 좌장: 나명수

Zeolites and the environmental issues

윤경병

서강대학교 화학과

Zeolites represent a large class of nanoporous crystalline inorganic materials whose frameworks consist of Si, Ge, Al, P, Ga, and many transition metals such as Ti, V, Co, Mn, Fe. The nanopores are often called cages or channels, depending on the shape of the pores, and they are normally filled with charge-balancing cations and water. Among various classes of zeolites, aluminosilicate zeolites have been most widely studied and applied in various fields. The framework of an aluminosilicate zeolite is formed by three-dimensional networking of $[AlO_4]^{5?}$ and $[SiO4]^{4?}$ tetrahedra via bridging oxygen atoms. As each aluminum atom has an excess negative charge, charge-compensating cations must be introduced into the structure, and they exist in the nanopores. Na^+ is the most common charge-balancing cation. The charge-balancing cations can be readily substituted with a variety of other cations via conventional aqueous ion exchange. By this way, various metal ions can be introduced into the zeolites. Protons (H^+) are also frequently exchanged into zeolites. So far, zeolites have been widely used catalysts, sorbents, ion exchangers, molecular sieve membranes, hosts for naked submicron quantum dots, hosts for nonlinear optical materials, building blocks for organized microcrystals, and so on. In this talk, our efforts to apply zeolites to remediate the contaminated environment will be presented. These efforts include the effective capture of the radioactive iodine molecules, radioactive Cs^+ and various heavy metal ions such as Hg^{2+}, Pb^{2+}, Cd^{2+}, Zn^{2+}, Cr^{3+}, and Tl^+. Also included will be the effective capture of CO_2 and NO by zeolites, and many others.

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Designed Synthesis and Assembly of Uniform-sized Nanoparticles for Medical and Energy Applications

현택환

서울대학교 화학생물공학부

Recently our group has been focused on medical applications of various uniform-sized nanoparticles. For example, using 3 nm-sized iron oxide nanoparticles, new non-toxic MRI contrast agent was realized for high resolution MRI of blood vessels down to 0.2 mm, which can be potentially applied to early diagnosis of cancers, stroke, and cardiovascular diseases. We demonstrated that ceria nanoparticles could protect against ischemic stroke in an in vivo animal model. In animal trials, intravenously administered ceria nanoparticles considerably reduced the stroke volume and nerve damage. We reported the first successful demonstration of high-resolution in vivo three-photon imaging using biocompatible and bright Mn^{2+} doped ZnS nanocrystals. Tumor vascular lining could be visualized with a resolution as small as 2 micrometer, which can be eventually applied to real-time monitoring of tumors during cancer surgery.We reported the large-scale synthesis of magnetite nanocrystals imbedded in a carbon matrix and hollow iron oxide nanoparticles. These iron oxide-based nanomaterials exhibited very high specific capacity and good cyclability. We demonstrate galvanic replacement reactions in metal oxide nanocrystals. When Mn_3O_4 nanocrystals were reacted with iron(II) perchlorate, hollow box-shaped nanocrystals of $Mn_3O_4/\gamma\text{-}Fe_2O_3$ (“nanoboxes”) were produced. Because of their non-equilibrium compositions and hollow structures, these nanoboxes exhibited good performance as anode materials for lithium ion batteries.

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Morphology-property correlation from highly conjugated molecular crystals

최희철

포항공과대학교 화학과, Center for Artificial Low Dimensional Electronic Systems, IBS

During the last two decades, remarkable advancement in physical science has been achieved by the discovery of quantum size effect (QSE) that grants new optical, electrical and chemical properties upon the reduction of sizes of bulk materials into low-dimensional particles of which energy states closely mimic those at molecular level. Similar achievements with comparable degree of importance are also plausible by structuring individual ensemble molecules into specific morphological structures in various dimensions, which demonstrate ‘morphology-property correlation’. Among several synthetic methodologies resulting in morphology-controlled crystallization of highly conjugated molecules[1,2], I will introduce two solution-based methods[3,4]: 1) drop-drying method and 2) solvent vapor crystallization (SVC) method. The drop-drying method is a very simple and fast process to obtain 1D or 2D structures of conjugated molecules in a solvated form. The examples include C60 molecules self-crystallized into 0D dots, 1D wires and 2D disks by simply dropping and drying several aliquots of C60 solution on a solid substrate. The determinant of the final geometry turns out to be solvent, of which geometry eventually guides C60 molecules to self-crystallize into specific geometries. One drawback of drop-drying process is that most of the resulting products are lying on a substrate, which limits its versatility especially when one needs to self-crystallize target molecules into vertical direction. Recently, we have succeeded in vertical self-crystallization of C60 molecules by SVC method of which experimental process resembles that of solvent vapor annealing (SVA) process.[5] More details about the growth mechanism of SVC process and potential applications will be discussed. Reference[1] Park. J. E.; Son, M.; Hong, M.; Lee, G.; Choi, H. C. Angew. Chem. Int. Ed., 2012, 51, 6383.[2] Shin, H. S.; Yoon, S. M.; Tang, Q.; Chon, B.; Joo, T.; Choi, H. C. Angew. Chem. Int. Ed. 2008, 47, 693?696.[3] Park, C; Yoon, E.; Kawano, M.; Joo, T.; Choi, H. C. Angew. Chem. Int. Ed. 2010, 49, 9670.[4] Park, C.; Song, H. J.;

Choi, H. C. Chem. Commun. 2009, 4803?4805.[5] Kim, J.; Park, C.; Park, J. E.; Chu, K.; Choi, H. C. ACS Nano 2013, 7, 9122-9128.

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발표코드: **INOR1-6**

발표분야: Past, Present and Future of Inorganic Chemistry in Korea

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Design and Synthesis of Metallic Nanogap Structures with Controllable Plasmonic Properties and Their Biosensing Applications

남좌민

서울대학교 화학부

Designing, synthesizing and controlling plasmonic nanostructures such as Au and Ag nanoparticles (AuNPs and AgNPs) with high precision and high yield are of paramount importance in chemistry, optics, nanoscience, materials science and nanobiotechnology. It is particularly important to generate and control ~1-nm plasmonic gap because the plasmonic gaps of ~1 nm or less can generate exponentially stronger plasmonic coupling signals than >1-nm plasmonic gap structures. Among many examples of the use of plasmonic nanogap, surface-enhanced Raman scattering(SERS)-based signal amplification and bio-detection methods using SERS-active plasmonic nanoparticles (NPs) have been drawing significant interest, and it has been known that SERS effect is very intense when Raman dyes are located within ~1-nm inter-particle junction. Here, I will describe various DNA-based design and synthetic strategies to build up new types of plasmonic nanogap metal nanostructures with high structural controllability. The use of these plasmonic nanostructures including anisotropic nanostructures as excellent optical signal enhancement platforms in detecting biomolecules sensitively, quantitatively and specifically will be presented. Other biosensing applications of these plasmonic probes including plasmonic nanoprobe-tethered supported lipid bilayer system and gel electrophoresis-based bio-barcode assay for microRNA detection will be also shown and discussed in this presentation.

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Metal Hybrid Nanostructures:Synthetic Strategies and Catalytic Applications

송현준

한국과학기술원(KAIST) 화학과

Metal hybrid nanostructures are currently of interest, due to the fact that the effective use or large enhancement of unique metallic properties are expected from a synergetic combination with other components. In the case that multiple properties are simultaneously required, the hybrid structures with multiple components are definitely promising for the purpose. For instance, nanoscale electronic circuits have semiconductors as main components and metals as electronic connectors (or electrodes), and heterogeneous catalysts comprise metal nanoparticles as active materials and high surface area metal oxides as supports to stabilize the active nanoparticles. In order to generate such metal hybrid nanostructures in a well-defined manner, numerous synthetic parameters should be considered to make stable junctions between distinct components, including crystal packing energy, growth kinetics, surface energy and mismatch, and chemical conversion. For all parameters, knowledge from fundamental inorganic chemistry is particularly essential.In the present study, we introduce our synthetic strategy to generate well-defined metal hybrid nanostructures with some key parameters. The examples are presented in the cases of metal-metal, metal-metal sulfide and selenide, metal-silica and metal oxide, and metal oxide-metal oxide systems. In addition, some applications arising from the synergistic combination of the multiple components are proposed, such as gas-phase, organic, and photocatalytic reactions.

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발표분야: Past, Present and Future of Inorganic Chemistry in Korea

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LOW-VALENT METAL CHEMISTRY; NICKEL CARBON BOND

이윤호

KAIST 화학과

There has been a surge of interest in the chemistry of low-valent first?row transition metal complexes in recent years. This interest has been in part motivated by a desire to generate species possessing uncommon metal-to-ligand multiple bond(s) such as oxo, imide, carbyne and nitride via partial or complete group transfer. In this presentation, a particular study of such species will be presented to show their respective roles in small-molecule transformations that include, carbon dioxide transformation for ACS/CODH chemistry and carbon monoxide conversion as a key step for Fisher-Tropsch synthesis. To test the validity of hypotheses concerning nickel's crucial roles in the stepwise reduction of CO2 to CO and C-C bond formation, synthetic nickel model systems are needed. Such systems can test the chemical compatibility of nickel with various proposed intermediates, and the reactivity patterns of such species. A four coordinate (PEP)Ni-L scaffold (E = N or P) where the L site is occupied by ligands such as N2, CO, CO2 and COOR will be described. The systems accommodating terminally bound CO in the three formal oxidation states (nickel(0), +1, and +2) and their reactivity toward CO2 and electrophiles will be illustrated.

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43 years with Studies on Coordination Chemistry

백명현

서울대학교 화학부

In this lecture, 43 years of life as a chemist in coordination chemistry, studying from macrocyclic chemistry to material chemisty, will be briefly reviewed.

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Application of homogeneous and heterogenous catalysts in the petrochemical industry

이상익

SK 이노베이션(주) 화학연구소

In the petrochemical industry, cataysts are indispensable materials in the whole process. In petroleum refinery, heterogenous catalysts based on zeolite and metal oxides are used to provide basic chemical materials enomously. On the other, in the production of commodities and fine chemicals with high values, homegeneous catalysts based on organometallic compounds are applied. In this presenation, catalysts research activites (homogeneous and heterogeneous both) in SK innovation will be briefly introuduced.

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발표분야: Catalysis: Current Trends and Future Challenges
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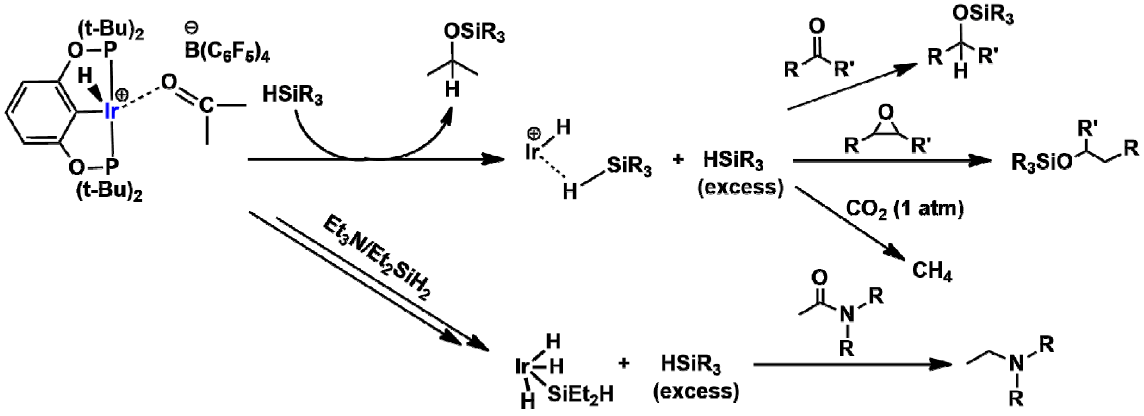
Well-Defined Iridium Silyl Complexes as Catalysts in Organic Transformations with Silanes: Scope, Limitation, and Mechanism

박세훈 David Bezier[1] Maurice Brookhart[1,*]

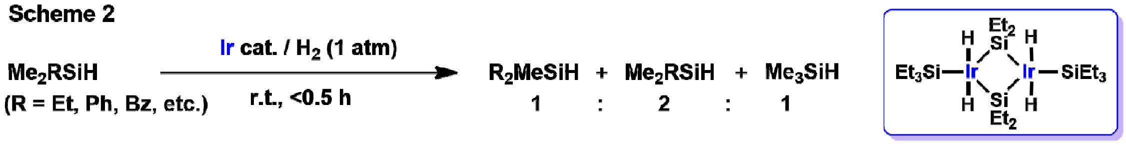
IBS 화학과 [1]University of North Carolina at Chapel Hill

The insertion process of Si-H moiety of silanes into functionalities such as carbonyls and olefins referred to as hydrosilylation is an extensively explored and widely used synthetic methodology in both academic and industrial fields of chemistry. This process provides an alternative to hydride reductions of various functional groups as well as a convenient one-step process for converting carbonyl compounds directly to protected alcohols. The most distinguishable feature in hydrosilylation would be catalytic process under mild conditions and easy tuning catalytic performance by choosing suitable silane. Despite of a number of highly promising metal catalysts for hydrosilylation in this context, iridium-based hydrosilylation catalysts are rarely explored, and hydrosilylation mechanisms remain less elucidated probably due in part to lability of metal silyl complexes as intermediates or active catalysts to be observed during catalysis. Recently, we have developed well-defined iridium silyl complexes, which in combination with hydrosilanes efficiently catalyze not only reduction of tertiary amides, alkyl ethers, and CO2, but also hydrosilylation of carbonyl functionalities and epoxides (Scheme 1). Herein we describe full account of reaction mechanism as well as scope and limitation in the iridium-catalyzed reductions with silanes. Additionally, we present here synthetic and unexpected mechanistic details of a highly efficient redistribution of simple trialkyl silanes, RR’R”SiH, catalyzed by a “ligand-free” dimeric silyliridum complex, in which the catalytic redistribution of silanes is initiated by a catalytic amount of H2 (Scheme 2).

Scheme 1



Scheme 2



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발표분야: Catalysis: Current Trends and Future Challenges

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Catalysts-Driven Technologies for Premium Polyolefins

전상진

LG화학 기술연구원 석유화학연구소

폴리올레핀 소재는 일상 생활용품에서부터 첨단 전자부품에 이르기까지 다양한 용도로 사용되고 있는 중요한 기초 소재이다. 전세계적으로 Dow 나 Exxon 을 비롯한 선진 기업들이 촉매 원천기술을 기반으로 범용제품을 탈피한 고부가가치 폴리올레핀 소재 개발을 주도하여 왔으며 국내에서는 20 여년 전 LG 화학이 처음으로 메탈로센 전담 연구팀을 구성한 이래로 비교적 짧은 기간 안에 독자적인 촉매 및 공정기술을 개발하고 상업화하여 현재 폴리올레핀 시장 전반에 걸쳐 메탈로센 기반 제품을 양산화하고 있다. 고부가가치의 폴리올레핀 제품 개발을 위해서는 제품 설계, 촉매 합성, 중합, 공정 기술 등이 서로 잘 융합되어야 가능한데, 이번 심포지엄에서는 LG 화학이 주도해 온 메탈로센 촉매기술 기반 제품들을 간략히 소개하고 현재 비중있는 관심을 가지고 연구 중인 메탈로센계 혹은 비메탈로센계 촉매에 관해 논하고자 한다.

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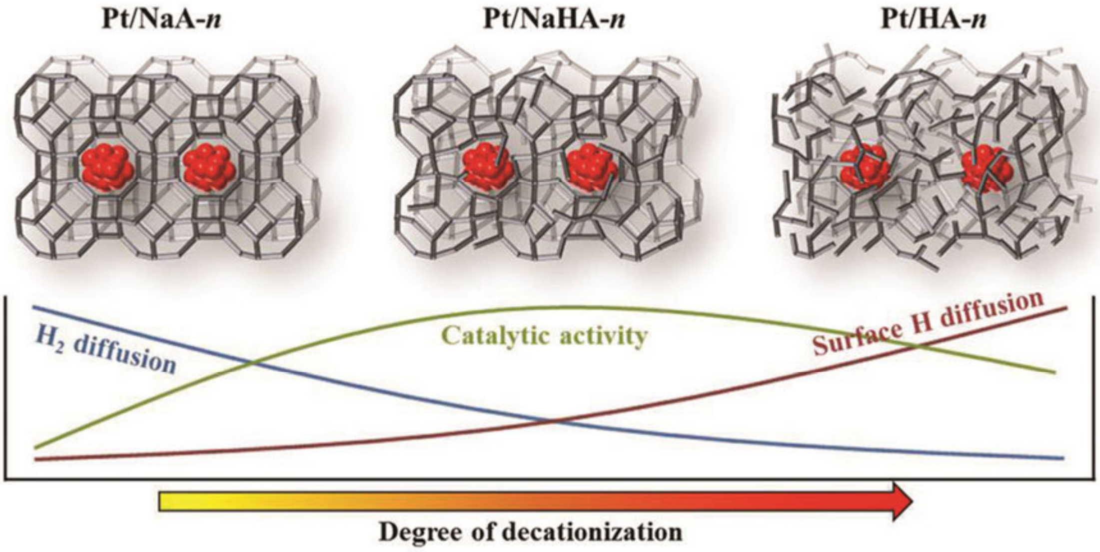
Understanding Catalytic Functions of Spillover Hydrogen with Well-Defined Model Catalysts

최민기

한국과학기술원(KAIST) 생명화학공학과

Hydrogen spillover has been extensively studied in catalysis field for several decades, but the nature and its catalytic functions still remain a topic of vigorous debate. Here we used well-defined Pt/LTA zeolite nanocrystals as a model catalyst for rigorously studying the catalytic functions of spillover hydrogen. LTA zeolite was chosen as a support for Pt clusters because the small pore aperture of the zeolite (0.4 nm) allows the selective diffusion of H_2 over organic molecules, which makes the catalytic interpretation very straightforward. We also deliberately control the zeolite crystallite size and the density of hydroxyl defect sites within the zeolite frameworks in order to study the effect of diffusion path length and the effect of defect sites on the migration of activated hydrogen. The results show that the presence of surface hydroxyls (*e.g.*, Bronsted acid) and external surface area of catalysts are the governing parameters for the catalytic use of spillover hydrogen. We propose a long-range H migration mechanism mediated by Bronsted acid sites based on quantum mechanical energetics. The spillover catalysts showed very high activities in hydrogenation/dehydrogenation, but virtually zero activities in hydrogenolysis. The distinct behavior indicates that the spillover and reverse spillover can be used for the addition and subtraction of H to or from organic molecules, but cannot break C-C bonds. It is reasonable to expect that the understanding on the catalytic functions of spillover hydrogen can be used to design advanced catalysts with enhanced catalytic activities, tolerance against thermal sintering and chemical poisoning, and distinct catalytic selectivity by choosing proper supports and metal encapsulation strategies.


Pt/NaA-*n*
Pt/NaHA-*n*
Pt/HA-*n*
H_2 diffusion
Catalytic activity
Surface H diffusion
Degree of decationization

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Nanostructure Design and Applications for Supported Metallic Catalysts

이현주

한국과학기술원(KAIST) 생명화학공학과

Heterogeneous catalysts have been widely applied in modern chemical industry. In spite of their practical importance, fundamental understanding and rational design of the heterogeneous catalysts has been impeded because the structure of the catalyst is often hard to control. We are trying to understand the chemical reactions occurred at the surface of nanoparticle catalysts and design the catalysts to have better performance of higher activity, selectivity, and stability. First, we control the shape of platinum-group metal nanoparticles to have specific facets, and tested them for electrocatalytic reactions or various hydrogenation reactions. The unique surface structure contributed to presenting higher activity and selectivity. The novel approach preparing shaped nanoparticles directly overgrown on the support with high surface area will be also introduced. Second, controlling the interaction between catalytic metal components and support materials can enhance activity and stability while minimizing the amount of precious metal catalysts. We found that the mode of Pt deposition on Au with different surface structure (e.g. Au(100) vs. Au(111)) is distinct resulting in different activity. The amount of deposited Pt on Au(111) surface was controlled and atomically dispersed Pt catalyst was prepared. This catalyst presented unprecedentedly high activity for electrocatalytic formic acid oxidation whereas the same catalyst showed no activity for electrocatalytic methanol oxidation.

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발표코드: **PHYS1-1**

발표분야: Frontiers in Physical Chemistry

발표종류: 심포지엄, 발표일시: 목 09:10, 좌장: 정연준

New Directions in the Self-Assembly of Functional Materials

George C. Schatz

Department of Chemistry, Northwestern University

Self-assembly of amphiphilic molecules provides a well-known way to make nanoscale (and larger) supramolecular structures including micelles, ribbons, sheets and aggregates. Recently there has been growing interest in the coupling of this self-assembly chemistry with silver and gold nanoparticles, leading to a new generation of materials of interest for optical devices and biodetection. And in another direction there is significant interest in the self-assembly of peptide amphiphiles to make biocompatible fibers that have useful functions. This talk describes the development of models for the assembly of these materials and for understanding a broad range of applications ranging from optical metamaterials to wound healing.

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One and Two Dimensional Coherent Spectroscopy: Theory and Experiment

조민행

고려대학교 화학과

Coherent IR and optical spectroscopy utilizing multiple femtosecond laser pulses has emerged as a promising technique enabling us to study structure and dynamics of complex molecular systems including biomolecules like proteins and nucleic acids as well as reactive molecules in condensed phases. Any complicated multidimensional spectroscopic technique can be designed by combining properly chosen components of excitation, propagation, and detection processes involving properly selected radiation-matter interactions. One of the most popular 2D IR or electronic spectroscopic methods is based on a four-wave-mixing technique. In such 2D optical spectroscopy, there exist a number of experimentally controllable variables such as frequencies of incident laser pulses, pulse-to-pulse delay times, relative optical phases, pulse propagation directions, polarization states, e.g., linearly, circularly, or elliptically polarized radiations, and polarization directions of the incident radiations. We have demonstrated that linear and nonlinear optical spectroscopy with a full control of incident radiation polarization states provides detailed insights into the structures of coupled multiple chromophore systems and parity-asymmetric property like molecular chirality in IR and visible frequency domains. In parallel with experimental applications of coherent multidimensional spectroscopy, we have developed classical and hybrid quantum and molecular mechanical simulation methods for a variety of linear and nonlinear vibrational response functions.

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Two Dimensional Molecular Electronics Spectroscopy for Molecular Fingerprinting, DNA Sequencing, and Cancerous DNA Recognition

김광수

울산과학기술대학교(UNIST) 화학과

Molecular spectroscopy has been widely used for identifying different molecules and compounds using various spectroscopy techniques like IR, Raman, and NMR. However, their use is often limited in nanoscience because of their resolution limit. Modulation of molecular orbitals in molecular systems is useful to tune the performance of electron/spin transport [1]. Electron/spin transport phenomena in molecular electronic/spintronic devices can be understood based on density functional theory (DFT) coupled to non-equilibrium Green function theory (NEGF) with which we have developed the Postrans program package [1,2]. We find that measuring two-dimensional conductance spectra of graphene nanoribbon (GNR) placed across a fluidic nanochannel leads to a fast DNA sequencing method [3]. As a single-stranded DNA (ssDNA) passes beneath the GNR, a single base interacts with the GNR via π-π stacking, giving a sharp conductance change due to Fano resonance. These unique resonance profiles reflecting the characteristic features and conformations of physisorbed molecules lead to two-dimensional molecular electronics spectroscopy (2D MES) [3,4]. The differential conductance with respect to bias and gate voltages not only distinguishes different types of nucleobases for DNA sequencing but also recognizes cancerous methylated nucleobases. This new 2D MES could open an exciting field to recognize single molecule signatures at atomic resolution. The advantages of the 2D MES over the 1D current analysis can be comparable to those of 2D NMR over 1D NMR analysis.[1] W. Y. Kim et al. Acc. Chem. Res. 43, 111 (2010).[2] W. Y. Kim et al. Nature Nanotech. 3, 408 (2008).[3] S. K. Min et al. Nature Nanotech. 6, 162 (2011). [4] A. C. Rajan et al. ACS Nano (2014). (in press). DOI: 10.1021/nn4062148

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Fundamental Processes of Photocatalysis of Methanol and Water on TiO2(110): A New Perspective on Photocatalysis

Xueming Yang

Dalian Institute of Chemical Physics, Chinese Academy of Sciences

Heterogeneous photocatalysis is a very important area of research and has received great attentions from chemists, physicists as well as material scientists because of its important applications in energy and environmental sciences and technologies. For many years, surface photocatalysis was viewed as an electron or hole driven event. However, the detailed physical picture of how a specific surface photocatalytic reaction takes place remains unclear. During the last few years, we have developed a series of new experimental tools (2PPE, TOF-TPD and STM) in our laboratory to investigate photocatalysis of methanol and water on TiO2(110) under well defined experimental conditions. Using these techniques in combination with laser-surface photocatalysis, we have investigated the fundamental processes of photocatalysis of methanol and water on TiO2(110). Important insights on the dynamics of surface photocatalysis have been derived from these experimental studies. In this talk, I will try to present these the new experimental results and my new perspective on the dynamics of surface photocatalysis.

일시: 2014년 4월 16~18일(수~금) 3일간

장소: 일산KINTEX

발표코드: **PHYS1-5**

발표분야: Frontiers in Physical Chemistry

발표종류: 심포지엄, 발표일시: 목 11:10, 좌장: 이영민

Can we determine the molecular structures by using an optical microscope?

김동호

연세대학교 화학과

By using single-molecule defocused wide-field imaging techniques and vector calculations, we have directly measured the position of transition dipole moments, angle differences between chromophores and consequently, determined the molecular structures of a series of acetylene-linked perylene bisimide (PBI) macrocycles with different ring size composed of three to six PBI dyes. Our findings illucidate that the structures of cyclic PBI arrays become distorted with increasing the ring size. We believe that the first direct observation of the molecular structures and heterogeneities of PBI macrocycles pave a new way towards understanding the structure-property relationship in a series of cyclic PBI arrays for further applications.

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발표코드: **PHYS1-6**
발표분야: Frontiers in Physical Chemistry
발표종류: 심포지엄, 발표일시: 목 11:35, 좌장: 이영민

Generation of reproducible MALDI spectra and its application to peptide quantification

김명수

서울대학교 화학부

It has been widely accepted by practitioners of MALDI that mass spectra generated by this technique are irreproducible, from sample to sample, from spot to spot in a sample, and from shot to shot in a spot. By serendipity, we observed that the spectral change, both in the pattern and in the abundance of each ion, occurred systematically. The way the spectra change and our interpretation of the change will be presented. The method to acquire reproducible spectra throughout a measurement will be presented. Its potential utility such as in protein quantification will be also presented.

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장소: 일산KINTEX
발표코드: **PHYS2-1**
발표분야: Physical Chemistry at the Nanoscale
발표종류: 분과기념강연, 발표일시: 목 13:25, 좌장: 이영민

Interaction of NO with Heme Proteins Probed by Femtosecond IR Spectroscopy

임만호

부산대학교 화학과

Nitric oxide (NO), a key cellular signaling molecule in many biological systems, regulates and mediates diverse processes. NO-bound heme adducts are observed frequently in various biological processes that involve NO signaling. Unlike CO and O_2 that bind only ferrous heme, NO can bind to both ferrous and ferric hemes, which contributes to a number of biological functions of NO in vivo. The rebinding dynamics of NO to various heme proteins after the photolysis of NO-bound adducts has been probed to reveal the NO-binding mechanism and to elucidate how the binding of NO to heme proteins is controlled by the structure and dynamics of proteins. The geminate rebinding (GR) of NO to ferrous-heme proteins is extremely efficient and proceeds on picosecond time scales, which has been attributed to the high reactivity of NO toward the Fe(II) of the heme. Nitrosylated ferric heme is autoreduced readily to the more stable Fe(II)?NO adduct but it is stabilized in NO-carrier heme proteins where maintaining the Fe(III) oxidation state is crucial for efficient NO delivery. Density functional theory calculations have shown that a NO-bound ferric model heme has a low-spin Fe(III)?NO(radical) state that might be critical for efficient NO transport by NO-carrier heme proteins. The elusive R state was investigated after photoexcitation of NO-bound ferric heme proteins using femtosecond time-resolved vibrational spectroscopy. Experimental findings will be presented in the conference.

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장소: 일산KINTEX
발표코드: **PHYS2-2**
발표분야: Physical Chemistry at the Nanoscale
발표종류: 분과기념강연, 발표일시: 목 13:45, 좌장: 이영민

Computational Chemistry at work: Quantum Computing to Neurodegenerative Diseases

신석민

서울대학교 화학부

Understanding the properties and the changes of materials at the molecular level is the essence of chemistry. Computational chemistry, aided by the recent developments in high speed and large capacity computer technologies, can provide direct and detailed information by mimicking the structures and motions of the real molecular systems. In this talk, we will introduce few examples where theoretical and computational approaches are adopted to provide basic understanding for operational principle of quantum computing and molecular mechanism of neurodegenerative diseases. Ability to actively control quantum states is crucial for constructing universal quantum computation. Novel quantum control schemes using strong lasers, based on adiabatic passages assisted by dynamical Stark shift, will be described. Investigating the formation of amyloid fibrils and prefibrilar aggregates of misfolded proteins is very important to elucidate possible causes for various neurodegenerative disorders. Systematic molecular dynamics simulations have been performed on the formation of the oligomers of Aβ peptide and peptides from α-synuclein. The general mechanism of amyloid formation and possible application to the designing new functional bionanostructures will be discussed.

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장소: 일산KINTEX

발표코드: **PHYS2-3**

발표분야: Physical Chemistry at the Nanoscale

발표종류: 심포지엄, 발표일시: 목 14:05, 좌장: 장준경

Perfect Crystal Gold Nanowires: their physical properties and biological/medical application

김봉수

한국과학기술원(KAIST) 화학과

Perfect crystal Au nanwoires (NWs) are superstrong, superelastic, and superplastic. They have diverse applications:i) nanoinjector: The Au NW was employed as a nanoinjector to deliver DNA directly into a cell nucleus by applying an electric pulse of ~1 V at a specific time, to the specific position and of a specific amount. These were verified by the expression of green fluorescent protein.ii) medical nanoelectrode: It was possible to record neural signals from a single neuron immediately after implanting Au nanoelectrodes into a mouse brain. This nanoelectrode produces little damage to the brain tissue with its size ~ 1/100 of the smallest electrode reported so far. This electrode has high signal-to-noise ratio and high spatial resolution. In the light of these features, Au nanoelectrodes can play an important role in the treatment of Alzheimer's disease and the researches for brain-machine interface, brain mapping, etc.iii) nanoelectrode as single-cell probe: It was possible to apply electrical stimulation to a single cell by using a Au nanoelectrode and to electrochemically monitor the consequent dopamine release from the cell in real time by using another Au nanoelectrode.iv) nanoantenna: Since single-crystalline Au/Ag NW has an ultraflat surface, surface plasmon can propagate to a very long distance. Employing that, multiple wavelength resonance is possible, which we observed on a Ag NW

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장소: 일산KINTEX
발표코드: **PHYS2-4**
발표분야: Physical Chemistry at the Nanoscale
발표종류: 심포지엄, 발표일시: 목 14:30, 좌장: 장준경

A molecular simulation study for the deformation and conductivity of nano-fibers aimed for a stretchable electronics

성봉준* 조현우 김정민

서강대학교 화학과

The effect of mechanical deformation of nano-fibers on the electrical conductivity is investigated by employing molecular simulations. The nano-fibers consist of polymers and carbon nanotubes, which are modeled using coarse-grained models. The conductive polymer fiber has been an issue of interest for its potential application to a stretchable electronics such as wearable devices and artificial muscles. However, the electrical conductivity of the polymer-based stretchable electronics decreases significantly during the deformation, which may limit the applicability of the polymer/CNT fiber for the stretchable electronics. Moreover, its physical origin for the decrease in electrical conductivity has not been explained clearly. Not surprisingly, in our simulations the electric conductivity decreases during the elongation of the polymer/CNT fiber. We employ a critical path approximation (CPA) find that the structure of the electrical network of the CNTs changes collectively during the elongation of the fiber, which accounts for the reduction of the electrical conductivity of the polymer/CNT fiber. We also compare our simulation results to recent experiments for the orientation and density correlation of CNTs in fibers.

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장소: 일산KINTEX

발표코드: **PHYS2-5**

발표분야: Physical Chemistry at the Nanoscale

발표종류: 심포지엄, 발표일시: 목 15:05, 좌장: 장락우

Novel Plasmonic Nanoarchitectures: Nanocrystals with High-Index Facets

한상우

한국과학기술원(KAIST) 화학과

The morphology of metal nanocrystals explicitly determines their plasmonic, electrical, and catalytic characteristics. Accordingly, numerous synthesis strategies have been developed for preparing metal nanocrystals with well-defined geometries, and for their hybridization with other nanomaterials. Here, facile fabrication processes of novel plasmonic nanoarchitectures using plasmonic metal nanocrystals with unprecedented morphology for efficient SERS and solar energy conversion platforms are reported. In the first part of talk, a facile aqueous synthesis process for the fabrication of Au nanocrystals with an unprecedented hexoctahedral structure enclosed exclusively by high-index {321} facets and their enhanced plasmonic properties and higher SERS activity than low-index-faceted Au nanocrystals are presented. In the second part of talk, the synthesis of heteronanocrystals by the local coupling of semiconductor with hexoctahedral Au nanocrystals and their excellent photocatalytic performance originating from the generation of strong electric field at the interconnecting junction between Au and semiconductor are presented.

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발표분야: Physical Chemistry at the Nanoscale
발표종류: 심포지엄, 발표일시: 목 15:30, 좌장: 장락우

Optical and Electrical Properties of Semiconductor Nanocrystal Solids

심은지

연세대학교 화학과

We investigate the optical and electrical properties of semiconductor nanocrystal solids. A new formula is introduced for predicting the carrier mobility of nanocrystal arrays as a function of the properties of quantum dots and capping ligands. As the quantum dot size decreases to a nanometer scale, conventional theories that are developed for bulk systems, such as Fermi's Golden rule and Marcus theory, fail to provide the correct trend of size-dependent rate constants. We discuss the non-monotonic electron and hole mobility trend in nanocrystal arrays, where non-monotonic behavior has been observed. Control of carrier mobility is crucial for application of nanocrystal solids and, thus, it is important to define the crossover diameter, where the carrier mobility reaches its maximum, with respect to the system properties. We also discuss optical properties of quantum dots that are contrary to the common understanding of band gap and size dependence.

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장소: 일산KINTEX

발표코드: **PHYS2-7**

발표분야: Physical Chemistry at the Nanoscale

발표종류: 심포지엄, 발표일시: 목 15:55, 좌장: 장락우

Nano-Plasmonics for Single-Molecule Photochemistry and Chemical Microscopy

김지환

서울대학교 화학과

I will present my research group's recent investigation on how the localized plasmon of a nanoparticle interacts with another plasmon, and with nearby molecules. The talk will cover three different yet related topics. First, I will demonstrate the use of scattering-type scanning near-field microscopy (s-SNOM) to directly visualize the capacitive / conductive coupling in dimeric nanoparticles and heterometallic nanorods. Second, I will talk about the use of gap-plasmons to locally induce photochemical reactions, and to follow chemical kinetics of individual organic molecules using the surface-enhanced Raman scattering (SERS). As a last topic, I will talk about the use of near-field coupling between a scanning probe and graphenes to visualize / identify the stacking domains (e. g., ABA versus ABC-type stacking in triple layer) hidden in multilayer graphenes.

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장소: 일산KINTEX

발표코드: **ANAL1-1**

발표분야: Advanced Bio and Environmental Analysis I: Sensor and Chip

발표종류: 심포지엄, 발표일시: 목 09:20, 좌장: 이혜진

Versatile Chip-Based Analytical Platforms Functionalized with Dendrimer-Encapsulated Nanoparticles

김주훈

경희대학교 화학과

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

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장소: 일산KINTEX

발표코드: **ANAL1-2**

발표분야: Advanced Bio and Environmental Analysis I: Sensor and Chip

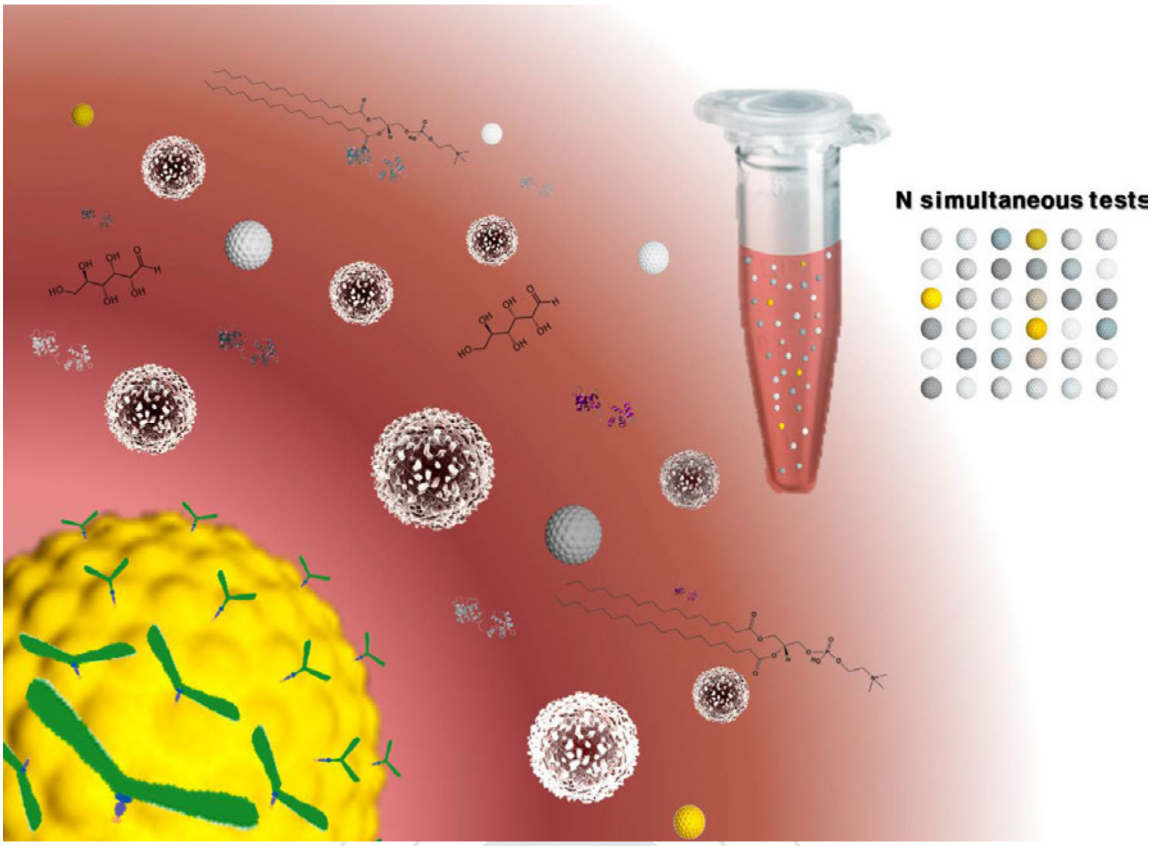
발표종류: 심포지엄, 발표일시: 목 09:45, 좌장: 이혜진

DC impedance based Cell Counting and Gold Microshells as 3D Suspension Array

정택동

서울대학교 화학부

Handling ions in microfluidic systems is a strong way to create unprecedented opportunities at the interface between informational technology and biotechnology. This presentation will be dealing with how a simple and well known polyelectrolyte can play creative roles in introducing electrochemical methods to microfluidic chip systems. A few novel chip systems on the basis of polyelectrolytic gel electrodes(PGE), including counters of blood cell and lethal bacteria based on DC impedance. Conductance across a pair of PGEs proportionally responds to the volume of micrometer scale objects that pass along the microchannel, e.g. the human blood cells and the functionalized microbeads. The same structure can lead to an efficient enrichment that makes very low concentration of proteins in human sera. In particular, gold thin shell covering the polymeric core can markedly minimize non-specific adsorption of albumin and things other than the antigens associated with the antibodies immobilized on the gold surface. Gold microshells dispersed in human blood can be easily and quickly collected within a small volume to be screened by dual detectors based on DC impedance and fluorescence on a chip. It is notable that sophisticatedly decorated gold microshells are compatible with MALDI analysis that reveals the information about unlabeled proteins captured onto the gold. In this talk, a few examples of gold microshells as 3D suspension array will be introduced to suggest innovative advances in chemistry as well as bioanalytical devices.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장소: 일산KINTEX
발표코드: **ANAL1-3**
발표분야: Advanced Bio and Environmental Analysis I: Sensor and Chip
발표종류: 심포지엄, 발표일시: 목 10:10, 좌장: 이혜진

Ratiometric method for bio analysis using magnetic nanoparticles (MNPs) in ICP-MS

임홍빈

단국대학교 화학과

When various bio targets in the range of small molecules like antibiotics to large cells were analyzed using nanoparticles, sample treatment procedure was the most critical point for practical application. In this presentation, we introduced a ratiometric technique to improve the analytical performance of both treatment platforms, i.e., sandwich-type and non-specific extraction immunoreaction. In order to achive this purpose, various magnetic nanoparticles doped with various metals were synthesized for the extraction of the targets. Then the synthesized nanoparticles were used for magnetic separation to extract biomarkers and the doped metal was used as an internal standard for the ratiometric measurement of the tagged particle. This ratiometric method compensated for the particle loss in a magnetic separation and suppressed the signal fluctuation which increased the calibration linearity significantly. The developed analytical method improved analytical figures-of-merits when targets were determined by ICP-MS.

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장소: 일산KINTEX

발표코드: **ANAL1-4**

발표분야: Advanced Bio and Environmental Analysis I: Sensor and Chip

발표종류: 심포지엄, 발표일시: 목 10:45, 좌장: 강성호

Optofluidic Nanosensor: A New Paradigm for Early Disease Diagnosis

주재범

한양대학교 생명나노공학과

We report a highly sensitive surface-enhanced Raman scattering (SERS)-based immunoassay platform for the simultaneous detection of multiple biomarkers. For this purpose, various types of bio-functionalized metal nanoprobes have been fabricated and used as SERS detection probes. Depending on the chemical composition, their optical properties have garnered much attention in biological studies approaching molecular dimensions. In addition, a programmable gradient microfluidic device has been utilized for automatic bioassay. The utility of this platform was demonstrated by the quantitative immunoassay of various protein markers. The total assay time from serial dilution to SERS detection takes less than 30 min because all of the experimental conditions for the formation and detection of immunocomplexes can be automatically controlled inside the exquisitely designed microfluidic channel. Accordingly, this technique is expected to be a powerful clinical tool for fast and reliable diagnosis of intractable diseases.

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발표분야: Advanced Bio and Environmental Analysis I: Sensor and Chip
발표종류: 심포지엄, 발표일시: 목 11:10, 좌장: 강성호

Localized Surface Plasmon Resonance (LSPR) Biosensors Based on Metal Nanoparticles with the Design of Bioreceptors

김민곤

광주과학기술원(GIST) 화학과

Label-free biomolecular assay based localized surface plasmon resonance (LSPR) of noble metal nanoparticles enables simple and rapid detection with the use of simple equipment. Nanosized metal nanoparticles exhibit a strong absorption band when the incident light frequency is resonant with the collective oscillation of the electrons, which is known as the LSPR. Here we demonstrate localized surface plasmon resonance (LSPR) substrates such as plasmonic Au nanodisks fabricated by a nanoimprinting process and gold nanorod-immobilized surfaces and their applications to highly sensitive and/or label-free biosensing. To increase detection sensitivity various bioreceptors weree designed. A single chain variable fragment (scFv) was used as a receptor to bind C-reactive protein (CRP). The results of this effort showed that CRP in human serum could be quantitatively detected lower than 1 ng/ml. Aptamers, which were immobilized on gold nanorods, were used to detect mycotoxins. The specific binding of ochratoxin A (OTA) to the aptamer was monitored by the longitudinal wavelength shift of LSPR peak in the UV-Vis spectra resulting from the changes of local refractive index near the GNR surface induced by accumulation of OTA and G-quadruplex structure formation of the aptamer. According to our results, OTA could be quantitatively detected lower than 1 nM level. Additionally, aptamer-functionalized GNR substrate was quite robust and can be regenerated many times by rinsing at 70 OC to remove bound target. During seven times of washing steps, the developed OTA sensing system could be reusable. Moreover, the proposed biosensor exhibited selectivity over other mycotoxins with an excellent recovery for detection in grinded corn samples, suggesting that the proposed LSPR based aptasensor plays an important role in label-free detection of mycotoxins.

References

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일시: 2014년 4월 16~18일(수~금) 3일간

장소: 일산KINTEX

발표코드: **ANAL1-6**

발표분야: Advanced Bio and Environmental Analysis I: Sensor and Chip

발표종류: 심포지엄, 발표일시: 목 11:35, 좌장: 강성호

Graphene Biosensors

서태석

한국과학기술원(KAIST) 생명화학공학과

2D and 3D graphene nanomaterials have shown their unique optical, electrical and mechanical properties which could be ideally used for biosensors. In the first part, I will introduce the synthesis of monolayer graphene quantum dots (GQDs) and graphene oxide quantum dots (GOQDs) that have circular shape and diameter of less than 4 nm starting from graphite nanoparticles. The blue PL emitting GQD and the green PL emitting GOQD were demonstrated, and their optical properties were compared by means of PL, PL excitation, UV-vis absorbance, and time-resolved PL to understand the PL mechanism of the nano-sized graphene materials. Our proposed methodology allows the production of homogeneous and single-layered photoluminescent GQDs and GOQDs with high yield and high reproducibility, and the produced GOQDs were used for biosensing applications. Compared to 2D graphene structure such as graphene, graphene oxide (GO), 3D graphene structure has also attracted worldwide attention due to its enhanced specific surface area and high compression/aggregation resistance. Thus, the combination of the 3D structure and the intrinsic excellent properties of graphene synergistically functions, so a variety of applications of the 3D graphene including energy storage and catalyst supports seem promising. In this study, we have demonstrated the synthesis of 3D graphene microballs by using a microfluidic droplet generator. The GO solution was encapsulated in the droplets and underwent through the capillary compression to form the 3D structure. In addition, we could load metal ions or metal nanoparticles together with the GO solution, resulting in the nanoparticle-3D graphene hybrids, which could be used for the catalyst supporter and the polymer composites with core-shell structure.

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발표코드: **ANAL2-7**
발표분야: Advanced Bio and Environmental Analysis II: Spectrometry and Separation
발표종류: 분과기념강연, 발표일시: 목 15:40, 좌장: 김태영

Analytical Applications of Nanostructured Metal Surfaces

김종원

충북대학교 화학과

The fabrication of nanostructured metal surfaces has attracted intensive research interest due to their useful applications in heterogeneous catalysis, electrocatalysis, electroanalysis, and surface-enhanced Raman scattering (SERS)-based sensing. Among various methods for the fabrication of nanostructured metal surfaces, electrochemical methods provide a simple route to construct well-defined and solid hierarchical metal nanostructures. In this presentation, we introduce our recent efforts into the fabrication of nanostructured metal surfaces and their analytical applications. We prepared nanostructured metal surfaces based on two strategies: 1) a simple electrochemical deposition of metal nanostructures on a clean electrode surface in the absence additives and 2) anodization of Au to form nanoporous structures. Originating from their unique surface structures, the nanostructured metal surfaces were utilized in various analytical applications such as electrochemical sensors, SERS-active substrates, and laser desorption ionization substrates. A simple preparation of well-defined nanostructured metal structures would allow new opportunities in various areas utilizing metal-based nanostructured surfaces.

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발표코드: **ANAL2-1**
발표분야: Advanced Bio and Environmental Analysis II: Spectrometry and Separation
발표종류: 심포지엄, 발표일시: 목 13:00, 좌장: 정회일

Expanding Applications for AFM-based Infrared Nanospectroscopy

<u>Curtis Marcott</u>[*] Craig Prater[1] Qichi Hu[1] Michael Lo[1] Kevin Kjoller[1]

Light Light Solutions [1]Anasys Instruments

Atomic force microscope-based infrared spectroscopy (AFM-IR) has been developed in recent years providing extremely high spatial resolution chemical characterization and imaging. The technique isbased on the combination of a tunable infrared laser with an atomic force microscope that can locally map and measure thermal expansion of nanoscale regions of a sample resulting from the absorption of infrared radiation. Because the AFM probe tip can map the thermal expansion on very fine length scales, the AFM-IR technique provides a robust way to obtain interpretable IR absorptionspectra at spatial resolution scales well below the diffraction limit. The technique also provides simultaneous and complementarymapping of mechanical properties and has been widely and successfully applied to applications in polymers and the life sciences. Most previous AFM-IR measurements have been performed usingtotal internal reflection illumination from below the sample, generally requiring samples to be prepared as thin sections transferred to an IR transparent prism. We have recently extended the AFM-IR techniqueto work in a "top side illumination" configuration. The top side illumination enables a much broader range of samples to be measured and can in some cases dramatically simplify sample preparation. Using top side illumination we have been able to measure samples including semiconductors, metal films, geological samples and others.

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발표분야: Advanced Bio and Environmental Analysis II: Spectrometry and Separation
발표종류: 심포지엄, 발표일시: 목 13:25, 좌장: 정회일

Application of field-flow fractionation (FFF) for multidimensional characterization of nanostructures of biotechnological interest

이승호* 정회일1,* 최재영

한남대학교 화학과 1한양대학교 화학과

The functionality of nanostructures of biotechnological interest (‘bio-nanostructures’) plays a key role in many areas, including food, pharmaceutical and chemical industries as well as in purely biological systems. Fundamental properties of bio-nanostructures are the size, molar mass and their distributions. Methods for determination of those properties are in urgent demand in the field of nano/biotechnology. Few analytical methods are designed for general use in this area, yet there are demanding needs. Many of commonly used methods for characterization only provide information on average properties which limits the application of the results as virtually all bio-nanostructures are polydispersed. Furthermore, conformational and structural data over the entire size distribution of a sample is of fundamental importance for the understanding of the structure and behavior of bio-nanostructures. Real samples are usually highly complex to analyze and characterize as different analytes may be simultaneously present in the samples. The analytes also dramatically differ in origin, chemical composition and molar mass. The analytical problem then becomes too complicated to be faced as a single analytical problem, and requires a proper combination of analytical methods ? ‘multidimensional analysis’. Field-flow fractionation (FFF) is considered to be an excellent candidate to employ for development of multidimensional analytical protocols in the field of nano/biotechnology. FFF can be used as the first dimension in multidimensional protocols in which other dimensions are constituted of uncorrelated techniques for further characterization of nanostructures, such as light scattering (LS). This presentation will introduce some of examples on multidimensional analysis for separation and characterization of physicochemical properties (chemical composition, size, shape, surface charge and their distributions) of various bio-nanostructures by combining FFF with such techniques as LS and single particle ICP-MS.

일시: 2014년 4월 16~18일(수~금) 3일간

장소: 일산KINTEX

발표코드: **ANAL2-3**

발표분야: Advanced Bio and Environmental Analysis II: Spectrometry and Separation

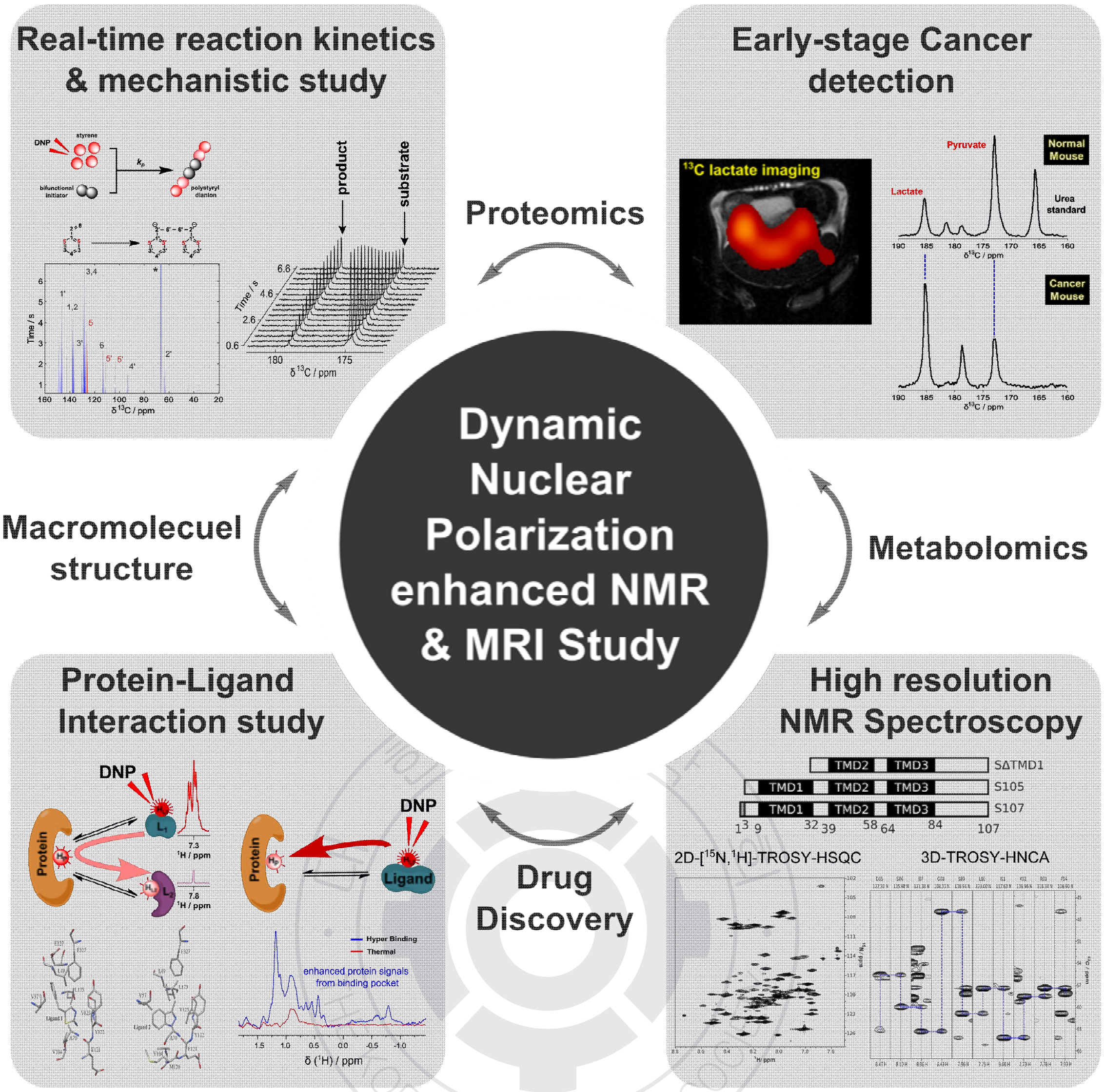
발표종류: 심포지엄, 발표일시: 목 13:50, 좌장: 정회일

Dissolution Dynamic Nuclear Polarization (DNP) Enhanced Magnetic Resonance Spectroscopy and Imaging

이영복

한양대학교 응용화학과

Nuclear magnetic resonance (NMR) spectroscopy is one of the most important analytical tools for organic and biological chemistry. It provides not only detailed information on the structure of small molecules and macromolecules, but also on molecular interactions. Because of the inherent low sensitivity of NMR, a long signal averaging time or a high spin concentration is often required. A variety of methods have been explored to improve the sensitivity of NMR. Especially, large signal gains can be obtained by hyperpolarization of the nuclear spins. NMR signals of hyperpolarized samples are enhanced by several orders of magnitude. Dissolution Dynamic Nuclear Polarization (D-DNP) is a versatile technique capable of polarizing many different nuclei in the solid state, and subsequently providing a hyperpolarized liquid sample following a dissolution step. The resulting signal enhancement has made it possible to obtain detailed information in research fields as varied as metabolic imaging or enzyme catalysis. This research aims to extend the applicability of D-DNP into new areas of chemistry, which involve the characterization of interactions and reactions involving large molecules.



Real-time reaction kinetics & mechanistic study

Early-stage Cancer detection

Proteomics

Macromolecuel structure

Dynamic Nuclear Polarization enhanced NMR & MRI Study

Metabolomics

Protein-Ligand Interaction study

Drug Discovery

High resolution NMR Spectroscopy

일시: 2014년 4월 16~18일(수~금) 3일간

장소: 일산KINTEX

발표코드: **ANAL2-4**

발표분야: Advanced Bio and Environmental Analysis II: Spectrometry and Separation

발표종류: 심포지엄, 발표일시: 목 14:15, 좌장: 정회일

Studies on Chemical Crosslink of Silicone Rubber

김현우

KCC 중앙연구소 분석팀

Crosslinks are junctions of elastomer strands in a three-dimensional network derived from curing technology (polymerization). Increased cross-linking gives an elastomer with increased modulus(stiffness) and decreased loss tangent(damping). The concentration of crosslinks is generally measured by the use of swelling method, elastic modulus method, and sol fraction. To elucidate the crosslinks of silicone elastomer, we have employed NMR and Silicon functionality test as well as sol fraction. NMR result shows that T1 and T2 relaxation time decrease with increase of crosslink density of the sample examined. This relationship is also compared to the GC data after silicon functionality test induced by the alkali cracking and sol fraction data. These methods provide a way to estimate the crosslinks closely related to mechanical properties of silicone elastomer.

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장소: 일산KINTEX

발표코드: **ANAL2-5**

발표분야: Advanced Bio and Environmental Analysis II: Spectrometry and Separation

발표종류: 심포지엄, 발표일시: 목 14:50, 좌장: 김태영

Supercritical fluid chromatography-tandem mass spectrometry for fast chiral separation of cetirizine in human plasma

엄한영 한상범*

중앙대학교 약학대학

A rapid and enantioselective analytical method has been developed and validated for the determination of levo-cetirizine in human plasma using supercritical fluid chromatography-tandem mass spectrometry (SFC-MS/MS). The SFC system provides high-throughput and unique selectivity compared with high performance liquid chromatography (HPLC). The cetirizine enantiomers have been separated by CHIRAL PAK IE column (2.1 mm x 150 mm, 5 µm particle size) which was maintained at 50°C. The isocratic mobile phase was composed of (A) carbon dioxide and (B) methanol with 5% (v/v) water in the proportion of 55:45 (v/v) at a flow rate of 0.85 mL/min. A stable isotope labeled internal standard, cetirizine-D4 was used. The tandem mass spectrometry was performed on an electrospray ionization source operating under positive ion mode and the analytes were detected using multiple reaction monitoring. The mass transitions of cetirizine and cetirizine-D4 were m/z 388.8→201.1 and 393.3→201.1. Analytical conditions of supercritical fluid chromatography such as column temperature, modifier content, additive content and flow rate were optimized using fractional factorial design and response surface methodology. Sample preparation was performed by SPE using HLB cartridge with ammonium formate buffer (20 mM, pH 3.0) and methanol. The dextro- and levo-cetirizine were well separated with no interference from endogenous plasma constituents in only 3.5 minutes. The developed method was validated in terms of linearity, accuracy, precision, recovery, limit of detection (LOD) and limit of quantification (LOQ). This analytical method was successfully applied to the analysis of pharmacokinetic study samples after oral administration of cetirizine to healthy Korean volunteers.

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장소: 일산KINTEX
발표코드: **ANAL2-6**
발표분야: Advanced Bio and Environmental Analysis II: Spectrometry and Separation
발표종류: 심포지엄, 발표일시: 목 15:15, 좌장: 김태영

Carbamidomethylation-based stable isotope labeling for quantitative determination of targeted shotgun proteomics

강덕진

한국표준과학연구원(KRISS) 삶의질측정표준본부

In quantitative shotgun proteomics, advanced mass spectrometry (MS) combined with diverse stable isotope labeling methods (e.g., ICAT, iTRAQ, mTRAQ, TMT, and etc.) has been considered as an effective solution in the determination of targeted protein(s) of interest and also offers the information of targeted protein-specific metabolic functions in a cell and pathogenically their interconnections with the virulence factors related to diverse diseases. But, these isotope-labeling strategies are unfortunately as challenging as ever, due to an irreproducible labeling caused by non-specific labeling of all hydroxyl residues of peptides. In this presentation, we introduce to a simple, ease-to-use, and inexpensive stable isotope labeling method for global quantitative proteomics, called as an isotope-coded carbamidomethylation (iCCM). In iCCM, the mass difference between each of light-/heavy-labeled protein sample was performed by means of which the two protein samples originated from two different states, for instance, healthy versus cancer sera, are individually isotopically labeled with iodoacetamide (IAA) and its isotope (IAA-$^{13}C_2$, D_2), respectively, that induces to a mass difference of + 4 Da at all cysteinyl residues in proteins. To evaluate the potentials of iCCM, we applied the developed iCCM to targeted quantification of human brain natriuretic peptide (BNP) as a biomarkers for a congestive heart failure, and also the quantitative profiling of lectin-specific serum N-glycoproteomics using an online mHFER-nLC-ESI-FT orbritrap-MS/MS. Based on our quantitative analyses, the developed iCCM-based isotope labeling can be considered as a complementary strategy for global quantitative proteomics with high reproducibility and robustness.

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장소: 일산KINTEX
발표코드: **BIO1-6**
발표분야: Lipid and Glycochemistry
발표종류: 분과기념강연, 발표일시: 목 11:10, 좌장: 유재훈

Synthetic Organic Molecules as a Powerful tool for the Functional Studies of Biomolecules

신인재

연세대학교 화학과

In post-genomic era, synthetic small molecules have been widely used as a powerful toolkit to elucidate the functions of proteins and carbohydrates in cells and living organism. As an effort for these studies, our group has developed various chemical tools to facilitate understanding of functions of biomolecules over last a decade. To evaluate functions of glycans, we have developed carbohydrate microarrays and chemical probes to detect glycan-binding proteins for functional glycomics. In addition, we have identified synthetic small molecules that affect neuronal differentiation and heart development for basic research and therapeutic applications. Furthermore, target-oriented drug delivery system has been exploited to selectively kill infected cells. In this presentation, I will discuss several chemical tools that have been developed by our group to provide valuable information on understanding of biological processes and novel drug discovery.

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장소: 일산KINTEX
발표코드: **BIO1-1**
발표분야: Lipid and Glycochemistry
발표종류: 심포지엄, 발표일시: 목 09:00, 좌장: 김경규

Chemical Synthetic Biology: Engineering the Biosynthetic Pathways of Natural Products

윤여준

이화여자대학교 화학나노과학과

We are mainly focusing on characterization of the biosynthetic pathway and creating the structural diversity of natural products including polyketides and aminoglycosides through the combinatorial biosynthetic approach. Synthetic biology is a new area of biological research that combines science and engineering in order to design and build novel biological functions and systems. Combinatorial biosynthesis is one area of synthetic biology for the generation of novel natural products. The basic concept of combinatorial biosynthesis is combining metabolic pathways in different organisms on a genetic level. The synthetic biological approaches combined with combinatorial biosynthesis will allow us “the biological total synthesis of natural products”, which will eventually lead to the unlimited structural diversification of natural product, drug discovery, and mass production. Some recent examples for this chemical synthetic biology approaches will be presented.

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발표분야: Lipid and Glycochemistry
발표종류: 심포지엄, 발표일시: 목 09:25, 좌장: 김경규

Nature's Unusual Chemistry:Switching Activity and Reaction Mechanism of Enzymes by Protein Engineering

Seung Seo Lee

School of Chemistry, University of Southampton

Since the seminal work by Sinnott and Jencks suggested the front-side (same face) nucleophilic attack in the glycosyl transfer reaction [1], the possibility of such unusual mechanism has been exercised in only a few occasions and very carefully [2,3]. Its possibility has been revoked to explain the seemingly unusual behavior of retaining glycosyltransferases [4]. Some of the crystal structures showed positioning of substrates, the leaving group and the nucleophile, in line with the proposed frontal face nucleophilic substitution mechanism, so called SNi or SNi-like mechanism [4]. Recently, we have provided experimental evidences supporting frontal face mechanism operating in a retaining glycosyltransferase, including kinetic isotope effects and linear free energy relationship [5] and the computational QM/MM metadynamics study [6]. These were supported by more experimental and computational studies of chemical and enzymatic glycosyl transfer [7, 8]. These studies suggest that an unusual SNi mechanism may be very much a reality and play an important role in the nature, considering that the importance of glycosyltransferases. The same unusual mechanism was found in an engineered retaining glycosidase, beta-glucosidase from Sulfolobus solfataricus (SSbG). When the catalytic nucleophile Asp of this enzyme was mutated to Tyr (E387Y), SSbG showed substantially low transglycosidation activity with retention of stereochemistry while its preference for substrates was switched. Most strikingly, kinetic studies of SSbG E387Y using mechanism-based inactivators showed that it did not involve the action of any nucleophile in its catalytic activity. Also, mutational studies indicated that SSbG E387Y did not require an enzymatic general acid/base residue. All of these are consistent with SNi-like mechanism. Computational studies supported the operation of SNi-like mechanism in the action of SSbG E387Y, yielding a feasible potential energy surface of the reaction coordinate. This is a showcase of major reaction mechanism switching from a double SN2 mechanism to a rare SNi mechanism by protein engineering and the first confirmation of the SNi mechanism in a beta-retaining glycosyl transfer reaction. Together, these comprehensive, experimental and computational data substantiate this unusual reaction mechanism in an enzyme. Its discovery in nature should prompt useful reassessment of many biocatalysts as well as their substrates and inhibitors.

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발표코드: **BIO1-3**
발표분야: Lipid and Glycochemistry
발표종류: 심포지엄, 발표일시: 목 09:45, 좌장: 김경규

O-GlcNAc as a Nutrient Sensor

조진원

연세대학교 융합오믹스 의생명과학과

Before Dr. Gerald Hart of Johns Hopkins University School of Medicine had discovered the existence of nuclear and cytosolic O-GlcNAc modification in 1984, complex carbohydrates were known to exist only in the endoplasmic reticulum, the Golgi apparatus and outside the cell, thus until now researches conducted on complex carbohydrates were limited to the endomembrane system. However, when O-GlcNAc modification was revealed to be closely involved with diabetes, Alzheimer’s disease and tumorigenesis, as well as that it competes against phosphatase for the modification sites on serine and threonine residues, the biological functions of O-GlcNAc modification, more specifically its role in cell signal transduction became the focal point of researches on molecular and individual levels. 3% of all glucose that enter the cell pass through the hexosamine biosynthesis pathway and are converted into UDP-GlcNAc. Utilizing UDP-GlcNAc as its substrate, O-GlcNAc modification is a modification unlike its predecessors in that its level is dynamically regulated by O-GlcNAc trasferase (OGT) which attaches O-GlcNAc onto target proteins, and reversibly removed by O-GlcNAcase (OGA). Proteomics and glycomics research technologies have determined that over 1,800 proteins are modified by O-GlcNAc, but due to a slowed development of technological infrastructure with which to recognize and study the function of O-GlcNAc modification, locating O-GlcNAc modification sites of a protein has only recently become an active field of research. There are only around 100 proteins of which the exact modified amino acid and its resulting functions are known ? a vastly small number compared to the number of proteins known to possess O-GlcNAc modification as aforementioned.

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발표코드: **BIO1-4**
발표분야: Lipid and Glycochemistry
발표종류: 심포지엄, 발표일시: 목 10:20, 좌장: 유재훈

Sphingolipid metabolism in cardiovascular and metabolic disease

박태식

가천대학교 글로벌캠퍼스 생명과학과

Overnutrition and sendentary lifestyle cause obesity in human. Ectopic accumulation of lipids in peripheral tissues and elevated free fatty acids are major causes of metabolic dysfunction. Lipotoxicity that accumulation of bioactive lipid metabolites disrupts the tissue function has been suggested for development of cardiovascular disease. Among them, ceramide has drawn attentions as a risk factor of cardiovascular and metabolic disease. Elevated ceramide derived from increased plasma free fatty acid leads to inhibition of insulin response, formation of atherosclerotic plaques, cardiomyopathy, and vascular dysfunction. Clinical studies have reported a positive correlation between ceramide/sphingomyelin and coronary artery disease. Intervention by pharmacological and genetic methods demonstrated that modulation of sphingolipid biosynthesis is a therapeutic target for these chronic diseases. The results obtained from animal models and pharmacological modulation elucidate the mechanism of alleviated cardiovascular dysfunction by reduced ceramide/sphingomyelin. Recent findings demonstrated that reduced ceramide improves vascular dysfunction caused by obesity via PP2A-mediated dephosphorylation of eNOS and reduced nitric oxide bioavailability. These results and those obtained from other disease models suggest that modulation of sphingolipids is a novel therapeutic method to prevent cardiovascular and metabolic dysfunction.

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발표코드: **BIO1-5**
발표분야: Lipid and Glycochemistry
발표종류: 심포지엄, 발표일시: 목 10:45, 좌장: 유재훈

Shotgun Lipidomics and Lipid MALDI Imaging of Brain Tissue

김영환

한국기초과학지원연구원 질량분석연구부

Lipids are essential cellular constituents that are multiple distinct yet critical roles as membrane bilayer, reservoirs for energy storage and the source of second messengers, in cellular function. The unique chemical structure of the majority of lipid molecular specie consists of linear combination of a small number of building blocks that include backbones, head groups, and aliphatic chains. Recently, shotgun lipidomics, to direct qualitative and quantitative analysis of complex mixtures of lipid by mass spectrometry have defined large-scale study, is a newly and rapidly expanding research field in system biology. Recent developments in imaging mass spectrometry (IMS) allow us to know the complete mapping of complex lipid mixture on tissue, including the identification of phospholipid and sphingolipid species at the molecular species level and their spatial distributions. In this study, lipids in mouse brain extracted with MTBE were analyzed by using microfluidic chip-based mass spectrometry, and UPLC/MS. They were identified at the molecular species level by a combination of ultra-high resolution MS profiling and ‘iLipid‘ program which was developed to search peak matching with lipid database. Their classification and fatty acyl compositions were also confirmed by using the precursor-ion scans of fragment ions specific to their polar head groups and neutral-loss scans of fatty acid carboxylate ions, respectively. The core focus was also given on optimization of MALDI imaging of lipids directly on brain tissue section. MALDI images of lipid molecular species on rat brain tissue obtained in the positive- and negative-ion modes show distinct anatomic structure of brain and indicate spatial distribution of individual lipid species over the tissue.

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발표코드: **BIO2-1**

발표분야: Fluorescent Probes for Bioimaging

발표종류: 심포지엄, 발표일시: 목 13:30, 좌장: 권영은

Fullerene-based fluorescent nanomaterials and their bioimaging applications

정진영

한국생명공학연구원(KRIBB) 바이오나노연구센터

Fluorescent nanomaterials are of great interest due to its unique physiochemical characteristics for versatile fields including biomedical applications such as biosensor/biochip, drug delivery, bioimaging, and therapy. Here, I will present studies on fullerene-based fluorescent nanomaterials and their applications in biosensor and bioimaging. First, fullerene-incorporated silica nanoparticles are synthesized by reverse microemulsion method and exhibit red photoluminescence, high photostability, easy penetration into live cells, and low cytotoxicity, all of which are essential properties for biomedical applications. Secondly, color-tunable fullerene nanoparticles were further synthesized by conjugating tetraethylene glycol using LiOH as a catalyst. The fluorescence of these materials was originated from electronic energy change causing chemical binding of silica or ligand. These nanomaterials are utilized in bioimgaing and fluorescent immunassay based on lateral flow strip biosensor.

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장소: 일산KINTEX
발표코드: **BIO2-2**
발표분야: Fluorescent Probes for Bioimaging
발표종류: 심포지엄, 발표일시: 목 14:00, 좌장: 권영은

Live cell imaging of proteins by intrinsic resonance energy transfer (iFRET)

정상전

동국대학교 화학과

Although fluorescence has offered invaluable detection methods of biological targets its biggest drawback is that requires inevitable labeling procedure on the target proteins, which may alter the inherent properties of the proteins. Furthermore, this procedure limits a range of the fluorescence-based cellular imaging application in artificial or engineered cell lines but not primary cells or tissues. Based on intrinsic fluorescence of the target proteins, intrinsic fluorescence resonance energy transfer (iFRET) has been developed via preparparation of target-specific probes by combining target-specific ligand with F?rster resonance energy acceptor (FREA) for tryptophan (Ex/Em = 280/350 nm). When the probe binds to the target protein FREA locates close to tryptophan, thereby facilitating FRET between tryptophan and FREA. We have tested and characterized various fluorescent molecules as iFRET acceptors, and applied for developing molecular probes specific to target proteins. The probes successfully detected the target proteins in purified forms as well as in cell lysate. We have also built a deep UV microscopy which can selectively excite free and protein-bound probes with 350 nm and 288 nm, respectively, and detect the signal at the same wavelength (emission wavelength of iFRET probe) thereby offering a chance for a spatiotemporal detection of target proteins such as enzymes or GPCR with high signal-to-noise ratio. In this symposium, we will present the principles and application of iFRET, and the structure and performance of deep UV microscope.

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발표코드: **BIO2-3**
발표분야: Fluorescent Probes for Bioimaging
발표종류: 심포지엄, 발표일시: 목 14:30, 좌장: 권영은

Construction of Biosensors under Live Cell Conditions by Chemical Protein Labeling

Itaru HAMACHI

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It is no doubt that protein is one of the key bio-macromolecules in many biological phenomena. Traditionally, analysis of proteins function has been conducted under the purified dilute aqueous conditions. However, it is now commonly recognized that functional and structural analysis of proteins in living cells is crucial for deep understanding of these molecules. Thus, development of chemical methods to selectively label, image and regulate a target protein under live cell conditions is now highly desired in the recent chemical biology research. I describe here our recent progress in chemistry-based methods for specific labeling of proteins driven by coupling of selective molecular recognition and reaction, so-called ligand-directed chemistry, under live cell conditions. In particular, I would like to discuss biosensor construction using proteins scaffold expressed in live cell on the basis of our ligand-directed chemistry. We believe that the new chemistry is expected to facilitate various aspects of fundamental chemical researches, in addition to diagnostic or pharmaceutical applications. References 1. Hayashi. T.; Hamachi, I. Acc. Chem. Res., 45, 1460-1469(2012).2. Takaoka. Y.; Ojida, A.; Hamachi, I. Angew. Chem. Int Ed., 52, Review 4088-4106 (2013).

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장소: 일산KINTEX
발표코드: **BIO2-4**
발표분야: Fluorescent Probes for Bioimaging
발표종류: 심포지엄, 발표일시: 목 15:20, 좌장: 정상전

Glutathione sensing and activation of "caged" PDT sensitizers

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Photodynamic therapy (PDT) is a noninvasive method of treating malignant tumors and age-related macular degeneration, and is particularly promising in the treatment of multidrug-resistant tumors. The PDT strategy is based on the preferential localization of certain photosensitizers in tumor tissues upon systemic administration. The sensitizer is then excited with red or near infrared (NIR) light, generating singlet oxygen ($^1O_2$) and thus irreversibly damaging tumor cells. Current practice of PDT is limited to a few functionalized porphyrins and related compounds, however these are not considered to be ideal photosensitizers for use in PDT. Among the limitations, the most prominent is the low extinction coefficient of porphyrins in the body’s therapeutic window (650?800 nm). As a consequence, many research groups worldwide are engaged in efforts to develop better sensitizers. One important aspect is the tight control of the delivery of cytotoxic singlet oxygen to be produced. This can be achieved by coupling sensing of a cancer related parameter to the singlet oxygen generation process. In an earlier design, we proposed a sensitizer which behaves as an “AND” logic gate. Singlet excited state of the sensitizer dye can take a number of different paths for de-excitation, through competing processes. Among these processes, photoinduced electron transfer (PeT), intersystem crossing (ic), fluorescence (fl), non-radiative de-excitation (nr) are the most prominent ones. Control of the relative rates of these processes can potentially offer new sensitizers with improved selectivity.Glutathione is an important cancer related intracellular species. We designed and synthesized caged photosensitizers which are inactive until they are acted upon by GSH. The methodology and potential of activatable photosensitizer design will be discussed. The financial support by TUBITAK (112T480) is gratefully acknowledged.References:'Designing Excited States: Theory-Guided Access to Efficient Photosensitizers for Photodynamic Action' Y. ?akmak, et al., Angew. Chem. Int. Ed., 2011, 50, 11937-11941. Cascading

of Molecular Logic Gates for Advanced Functions: A Self-Reporting, Activatable Photosensitizer' S. Erba?-?akmak, E. U. Akkaya, Angew. Chem. Int. Ed., 2013, 52, 11364 ?11368. Proof of principle for a molecular 1 : 2 demultiplexer to function as an autonomously switching theranosticdevice' S. Erba?-?akmak, et al., Chem. Sci., 2013, 4, 858?862.

일시: 2014년 4월 16~18일(수~금) 3일간
장소: 일산KINTEX
발표코드: **BIO2-5**
발표분야: Fluorescent Probes for Bioimaging
발표종류: 심포지엄, 발표일시: 목 15:50, 좌장: 정상전

Fluorescent Probes for HOCl and Biothiols

윤주영

이화여자대학교 화학·나노과학과

Fluorescence is an important detection method due to its simplicity and high detection limit. In this presentation, we focus our recent contributions to fluorescent chemosensors. Recently, we designed FBS as a new fluorescent HOCl probe which has high selectivity, sensitivity and short response time in a broad range of pH. Compared with other sensors, the “dual-lock” structure of FBS has an advantage of eliminating interferes from other ROS/RNS. Importantly, we further showed that our HOCl probe could be applied for the *in vivo* imaging of physiological HOCl production in the mucosa of live animals.We recently developed a novel strategy, which relies on changes in the π-electron conjugation length of cyanine molecules resulting in large emission shifts, has great potential for the creation of cyanine-based probes. The highly sensitive and selective, cyanine-based Zn^{2+} fluorescent sensor CTMPA was designed, prepared and utilized to monitor endogenous zinc ions in live cells and organisms. Particularly, CTMPA serves as the first probe for fluorescence detection of neuromasts in zebrafish. As a second example of cyanine based probe, we developed a highly selective ratiometric near-infrared cyanine-based probe CyAC for cysteine (Cys) over homocysteine (Hcy) and glutathione (GSH). CyAC was successfully applied for bioimaging Cys in living cancer cells.

일시: 2014년 4월 16~18일(수~금) 3일간

장소: 일산KINTEX

발표코드: **ORGN1-5**

발표분야: Current Trends in Organic Chemistry I: Supramolecular Chemistry & Molecular Sensors

발표종류: 분과기념강연, 발표일시: 목 11:20, 좌장: 김종승

Porphyrin-based functional materials

장우동

연세대학교 화학과

Porphyrins are a class of aromatic macrocycles that composed of four pyrrole subunits connected via methine bridges. Because of the large pi-conjugation area, porphyrins generally have distinct photophysical and electrochemical properties. Four nitrogen atoms in the porphyrin ring can chelate various metal ions. Therefore, the physical and chemical properties of porphyrins can be tuned by metal coordination into focal core. The symmetric architecture of porphyrins often utilized as a building block for the construction of functional supramolecular architecture. In this symposium, I would like to introduce several examples of bio-inspired application of porphyrin-based functional materials.

일시: 2014년 4월 16~18일(수~금) 3일간

장소: 일산KINTEX

발표코드: **ORGN1-1**

발표분야: Current Trends in Organic Chemistry I: Supramolecular Chemistry & Molecular Sensors

발표종류: 심포지엄, 발표일시: 목 09:00, 좌장: 김태우

"Action at a Distance" for Chemical Sensing and Switching: Torsional Control of Light-Emitting Properties and Chemical Reactivities

이동환

서울대학교 화학부

An increasing number of functional materials are built with π-conjugated chemical architectures. The practical utility of such constructs derives from rich optical and electrochemical properties that are inherent to their extended electronic structures, and the ability to manipulate them by either covalent or non-covalent synthetic modifications. Taking inspirations from the mode of operation of certain transmembrane protein complexes, we have devised a simple mechanical coupling scheme that correlates torsional motions of multiple aromatic groups that interact through a symmetric array of hydrogen bonds. The assembly and disassembly of multiple non-covalent contacts within such branched π-conjugation result in a dramatic switching of fluorescence properties. Taking this concept a step further, we are currently exploring stimuli-responsive chromophores and receptors, in which restricted torsional motions along the π-conjugated molecular backbone can be exploited for reactivity-based detection of biologically/environmentally relevant molecules and ions. In this presentation will be discussed the advent of this chemistry, its current progress, and future developments.

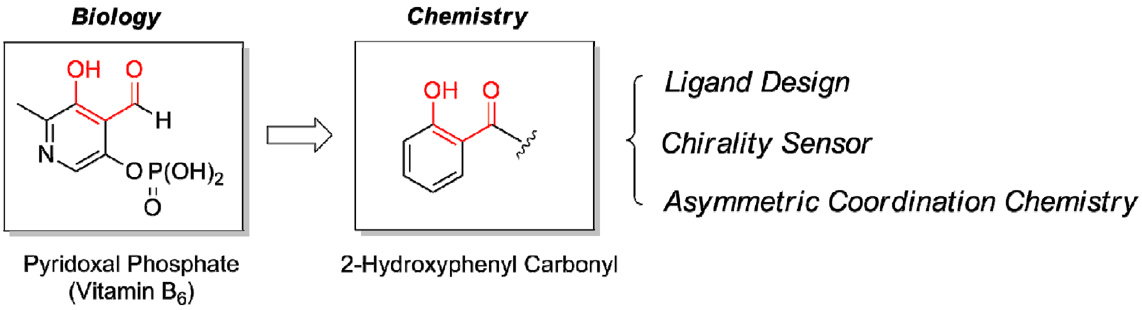
일시: 2014년 4월 16~18일(수~금) 3일간
장소: 일산KINTEX
발표코드: **ORGN1-2**
발표분야: Current Trends in Organic Chemistry I: Supramolecular Chemistry & Molecular Sensors
발표종류: 심포지엄, 발표일시: 목 09:30, 좌장: 김태우

2-Hydroxyphenyl Carbonyl: A Versatile Platform for Chirality Sensor and Ligand Design

김현우

한국과학기술원(KAIST) 화학과

Pyridoxal phosphate (Vitamin B_6, Figure), a cofactor in amino acid metabolism, includes the "2-hydroxyphenyl carbonyl" structure that plays an essential role in the catalytic cycle. In chemistry, salicylaldehyde is the simplest compound including the "2-hydroxyphenyl carbonyl" structure. SciFinder search shows that more than 20,000 publications have appeared with salicylaldehyde. One reason of its popularity is the existence of an internal hydrogen bond that affects the thermodynamics and kinetics of the reaction. Thus, the salicylaldehyde structure has found numerous applications in organic chemistry such as the development of catalysts and sensors. The well-known chiral salen ligands pioneered by Jacobsen and Katsuki are made by the reaction between diamines and salicylaldehyde derivatives. However, the other 2-hydroxyphenyl carbonyl compounds are somewhat ignored by synthetic chemists. We focused on the reactivity, stability, and geometry of this system and found some new applications: chirality sensor, asymmetric coordination chemistry, and ligand design. In this presentation, some of our recent results will be presented. The essential concepts and experimental details of these topics will be introduced.



Pyridoxal Phosphate (Vitamin B_6)

2-Hydroxyphenyl Carbonyl

일시: 2014년 4월 16~18일(수~금) 3일간

장소: 일산KINTEX

발표코드: **ORGN1-3**

발표분야: Current Trends in Organic Chemistry I: Supramolecular Chemistry & Molecular Sensors

발표종류: 심포지엄, 발표일시: 목 10:00, 좌장: 김태우

In Situ Generated Reactive Molecular Probes for Mapping Endogenous Protein-Protein Interactions in Living Cells

이현우

울산과학기술대학교(UNIST) 화학과

In a human cell, 18,000 different proteins are known to be expressed. These proteins are not evenly distributed in a cell but are very specifically localized in its targeted space to make various microenvironments by forming ultrastructures. In this session, a newly developed protein-protein interaction (PPI) mapping methods using in situ generation of reactive molecular probes for mapping localized protein complex in a living cell will be presented.

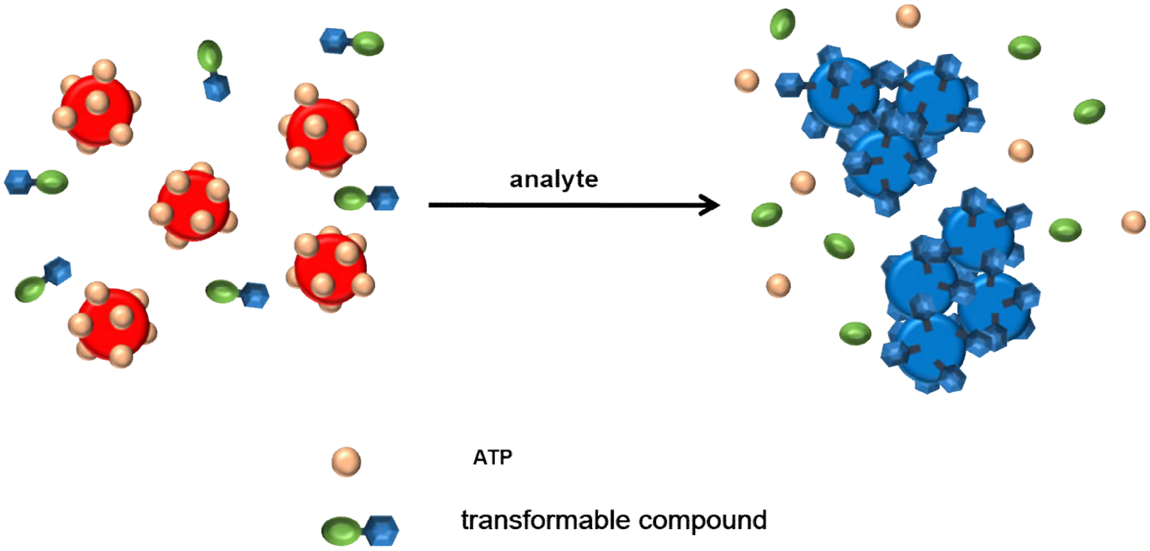
일시: 2014년 4월 16~18일(수~금) 3일간
장소: 일산KINTEX
발표코드: **ORGN1-4**
발표분야: Current Trends in Organic Chemistry I: Supramolecular Chemistry & Molecular Sensors
발표종류: 심포지엄, 발표일시: 목 10:50, 좌장: 김민

ATP stabilized gold nanoparticle based-colorimetric sensor and its application

한민수

중앙대학교 화학과

Gold nanoparticles (AuNPs) are ideal chromophores because they have 3-5 orders of magnitude higher extinction coefficients than organic dye molecules.10 Moreover, the unique distance-dependent optical properties of AuNPs can be chemically programmed through the use of specific host compounds, such as DNA, to induce a dramatic color change from red to blue. Due to their high extinction coefficients and distance-dependent optical properties, AuNP-based colorimetric sensors have been developed extensively to detect metal ions, proteins, DNA, and small molecules.Recently, several methods for stabilizing unmodified AuNPs in buffer systems with high electrolyte concentration have been reported; in these methods, the AuNPs are simply mixed with ATP.2 Unlike citric acid stabilized AuNPs, the AuNPs are stable over a wide range of buffer pH even in the presence of high concentrations of salt and protein. However, these stabilized AuNPs aggregate immediately when exposed to strong metal ligands such as thiol derivatives, iodide, and phenanthroline. With this information, we developed new type colorimetric sensor systems by combining transformable compounds to strong metal ligands and ATP stabilized AuNPs (sAuNPs). The compounds are unreactive with sAuNPs but these molecules can be changed to strong metal ligands when exposed to target analytes. The changed molecules react with the sAuNPs quickly and this process immediately induces color change from red to blue as scheme 1. This process is enabling to detect analyte with naked eyes, without resorting to a spectrometer. Scheme 1. A schematic representation of sensing mechanism for sAuNPs based colorimetric sensor


analyte
ATP
transformable compound

일시: 2014년 4월 16~18일(수~금) 3일간

장소: 일산KINTEX

발표코드: **ORGN2-1**

발표분야: Current Trends in Organic Chemistry II: Functional Organic Materials

발표종류: 심포지엄, 발표일시: 목 13:30, 좌장: 장우동

Mechanistic Studies of the SpnF-Catalyzed [4+2] Cycloaddition in Spinosyn A Biosynthesis

Hung-wen Liu

University of Texas, Austin, Texas, USA

SpnF is a polyketide tailoring enzyme in the biosynthetic pathway of the insecticide spinosyn A produced by Saccaropolyspora spinosa. SpnF is unique, because it is the only know enzyme that specifically catalyzes a [4+2]-cycloaddition without introducing any other changes to its substrate. The same cycloaddition also takes place nonenzymatically, but at a much reduced rate. If the reaction catalyzed by SpnF is a concerted process with a single pericyclic transition state, then SpnF would be the first example of a naturally selected Diels-Alderase. In order to investigate this possibility, α-secondary deuterium kinetic isotope effects were measured at both points of rehybridization in the diene during both the nonenzymatic and SpnF-catalyzed [4+2]-cycloaddition reactions. This was accomplished using regiospecifically deuterated substrates and electrospray ionization, time-of-flight mass spectrometry to follow changes in deuterium enrichment of the substrate as the reaction progressed. The presentation will describe the methodology and theory underlying the measurement of these KIEs, address the key challenges regarding these measurements and offer a mechanistic discussion of their implications for understanding the SpnF catalyzed [4+2]-cycloaddition.

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장소: 일산KINTEX
발표코드: **ORGN2-2**
발표분야: Current Trends in Organic Chemistry II: Functional Organic Materials
발표종류: 심포지엄, 발표일시: 목 14:00, 좌장: 장우동

FITGE-Based Target Identification for the Connection of Rational Drug Discovery with Phenotypic Screening

박승범

서울대학교 화학부

In this presentation, a systematic study of Seoul-Fluor will be presented. During our continuous efforts on the construction of drug-like small-molecule libraries using pDOS strategy, we aimed to develop a novel fluorescent core skeleton for the development of bioprobes, applicable for image-based screening. Guiding with computational simulation, we constructed a novel collection of fluorophores, which covers the full-color emission range with predictability. Seoul-Fluor analogs were successfully applied in HCS. Lastly, we developed a new target identification platform, FITGE, which aims to preserve protein-small molecule interactions under the intact cellular environment. After a series of failures using conventional target ID methods, we successfully identified the protein target of anti-proliferative compound with FITGE only under the live cell condition and observed the environment-dependent binding events of a functional small molecule by direct comparison between live cells and cell lysates. Even though it still requires the synthesis of bioactive probes with photo-crosslinker moiety, we believe our FITGE strategy can provide a unique technology platform for target identification in live cells.

일시: 2014년 4월 16~18일(수~금) 3일간
장소: 일산KINTEX
발표코드: **ORGN2-3**
발표분야: Current Trends in Organic Chemistry II: Functional Organic Materials
발표종류: 심포지엄, 발표일시: 목 14:50, 좌장: 박승범

Expanded Porphyrins Based on Pyrrole, Pyridine, and Furan

Jonathan L. Sessler

The University of Texas, Austin, USA

Expanded porphyrins are now a well-established class of macrocycles. They have seen application in areas as diverse as anion recognition and transport, liquid-liquid ion extraction, photodynamic therapy, and anticancer drug development. In recent years expanded porphyrins have helped increase our understanding of aromaticity and antiaromaticity. One approach to extending these latter frontiers involves making systems whose size, shape, and electronic structure is rigorously controlled. Another involves replacing the pyrrolic subunits typically found in expanded porphyrins with subunits, such as pyridine, that do not normally allow for through conjugation. In this lecture, an update on recent systems that have been synthesized and studied in our laboratories will be presented. Particular emphasis will be placed on systems that support unexpected electronic configurations, including unusual [4n +1] π-electron semi-aromatic peripheries. Several lead references are provided below.This work has benefited from support from the U.S. National Science Foundation, as well as the Robert A. Welch Foundation and the Korean World Class University program. Productive collaborations with a number of groups, including those of Profs. Christophe Bucher, Dirk Guldi, Pradeepta Panda, Changhee Lee, Jan Jeppesen, and Tomas Torres, are also gratefully acknowledged.

일시: 2014년 4월 16~18일(수~금) 3일간

장소: 일산KINTEX

발표코드: **ORGN2-4**

발표분야: Current Trends in Organic Chemistry II: Functional Organic Materials

발표종류: 심포지엄, 발표일시: 목 15:20, 좌장: 박승범

New Blue Phosphorescent Iridium Complexes for OLED

윤웅찬

부산대학교 화학과

We have conducted investigations to develop novel highly efficient deep blue phosphorescent (at ~ 440 nm) iridium complexes which might be useful for full color OLED displays and efficient WOLEDs. Iridium complexes attract continuous attention as emitting-dopant materials for OLEDs because of their phosphorescence emission of high quantum efficiency.

Based on the earlier reports[1] and observations[2], we designed new iridium complexes which contain 2-(2,4-difluorophenyl)-4-methylpyridine, 2-(2,4-difluoro-3-trifluoromethylphenyl)-4-methylpyridine, 2-(2,4-difluorophenyl)-4-methoxypyridine, 2-(2,4-difluoro-3-trifluoromethylphenyl)-4-methoxypyridine, and 2-(2,4-difluorophenyl)-2-N,N-dimethylaminopyridine as main ligands, and the new substituted 4-picolinates, 2-pyridyltriazolate derivatives, imidazole carboxylates of low HOMO and high LUMO energy level[3] as ancillary ligands.

Their structures were characterized by spectroscopy and single crystal x-ray diffraction. Their UV-vis absorption and emission spectra, electrochemical properties, and phosphorescent quantum yields were measured. As previously observed, CF_3 group substitutions at 5'-position of main ligands led to 8-10 nm hypsochromic shift[2] and CH_3 substitution on 4-position of pyridyltriazole ancillarty ligand resulted in further 8 nm hysochromic shift in emissions. N-Methylimidazoyl substitutions on 5-position of 3-(trifluoromethyl)-1,2,4-triazole in place of 4-methylprydyl allowed almost equivalent blue shifts in their emissions[4]. In the lecture will be discussed our rational design, synthesis, and characterization of new blue or deep blue phosphorescent iridium complexes for OLEDs applications.

References

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2. (a) Takizawa, S.; Echizen, H.; Nishida, J.; Tsuzuki, T.; Tokido, S.; Yamashita, Y. *Chem. Let.* 2006, 35,

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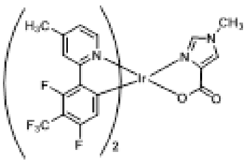
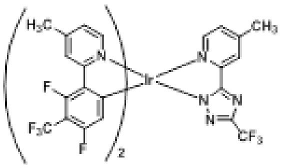
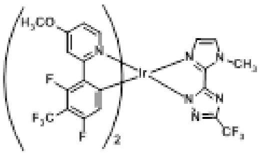


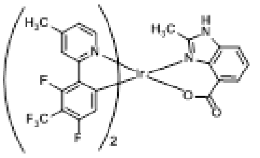
λ_{max}= 458nm, 483nm
ϕ = 0.80



λ_{max}= 448nm, 475nm
ϕ = 0.42



λ_{max}= 448nm, 474nm
ϕ = 0.60



λ_{max}= 459nm, 484nm
ϕ = 0.28

일시: 2014년 4월 16~18일(수~금) 3일간

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발표코드: **ORGN2-5**

발표분야: Current Trends in Organic Chemistry II: Functional Organic Materials

발표종류: 심포지엄, 발표일시: 목 15:50, 좌장: 박승범

Biomolecular Robotics for Chemomechanically Driven Guest Delivery Fueled by Intracellular ATP

Takuzo Aida

The University of Tokyo, Japan

Realization of “surgical nanomachines”, proposed by physicist Richard Feynman, is undoubtedly one of the ultimate scientific challenges. Such nanomachines are expected to detect particular biological (endogenous) signals and judge the necessary tasks to cure wounded tissues. Inspired by this vision, we developed the first robotic nanocarrier that senses ATP (adenosine-5’-triphosphate) and breaks up spontaneously to release a guest molecule. This unprecedented nanocarrier consists of tubularly assembled GroEL, a barrel-shaped chaperonin protein, ubiquitously present in the human body as an essential biomolecular machine that assists refolding of denatured proteins by trapping them inside its barrel. For GroEL to release refolded proteins from the cavity, it binds ATP, which is then hydrolyzed to create ADP, wherein GroEL undergoes a large conformational change. We took note of this ATP-fueled chemomechanical motion and hypothesized that if the mechanical force generated by this motion is large enough to cut non-covalent interactions, the tubular GroEL assembly may break up spontaneously into its monomer upon binding with ATP and release a guest molecule. We demonstrated that this idea works well. The nanocarrier has the potential to differentiate biological environments in terms of ATP concentration and release guests in ATP-rich regions. The concentration of intracellular ATP is in a range of 1?10 mM, while that of extracellular ATP is very low (~5 ?M), except around inflammatory tissues such as tumor tissues, where extracellular ATP concentrations are high at around 1 mM. We found that nanocarrier scission occurs with a sigmoidal dependency on ATP concentration, indicating a possibility of fail-safe operation.

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장소: 일산KINTEX
발표코드: **MEDI-1**
발표분야: Current Trend and Future in Metabolic Disease
발표종류: 심포지엄, 발표일시: 목 13:30, 좌장: 이광호

대사성 증후군 질환 치료제의 신약개발에서의 기회는?

박희동

LG생명과학 신약연구소

대사성 증후군은 metabolic syndrome 이라고 하며, 이는 심혈관 질환이나 당뇨병의 위험요인 증가시키는 고혈압, 고지혈증, 비만, 인슐린저항성 등을 한가지 질환 군으로 총칭하는 것이다. 특히 이들 질환 중에서, 고혈압의 경우는 신약개발의 큰 성공을 거두어, 사업적 기회가 더 이상 존재하지 않은 분야라 판단되며, 비만, 당뇨 및 고지혈증은 서로의 병인에 연관성이 깊으며, 식생활의 서구화, 운동부족, 개발도상국의 선진화, 노령화 사회의 도래로 대사성 증후군의 증가는 매우 심각한 질병으로 우리에게 다가 오고 있는 것은 주지의 사실이다. 지난 20 년간 세계적으로 대사성 증후군 환자가 폭발적으로 증가해 왔다. 향후 10 년간에도 이들 환자의 수는 다른 어느 질병보다 더 빠르게 증가 하리라 예측하고 있다. 최근 보고에 의하면 미국인의 25% 이상이 대사성 증후군에 속한다고도 한다. 따라서 대사성 증후군에 대한 신약시장은 어느 다른 분야보다 크며 향후 빠르게 성장할 것으로 예측하고 있다. 대사성 증후군 질환들은 21 세기 인류의 건강을 위협할 질병으로 간주되어 이를 치료 할 수 있는 신약의 개발이 그 어느 때보다 절실히 요구되고 있다. 이러한 환경 속에서 우리는 어떻게 미래를 준비해야 되는가를 생각해 볼 필요성이 있다고 생각 된다. 본 발표에서는, 현재 신약개발의 R&D 투자가 줄어들고, 사업적 성과 창출이 심히 우려되는 상황에서, “어떻게 효율적인 성장이 가능한 신약 R&D 방법론을 발굴하고, 한정된 자원 상황 속에서 어느 연구 분야에 집중할 것인가? 어떤 시장을 공략할 것인가?” 가 한국의 신약 개발 주체들에게 심각한 이슈로 다가오고 있다, 결론적으로 대사성 증후군 질환들 중에서 각 연구 주체들의 강점을 더욱 강화하고, 오픈 이노베이션을 포함한 새로운 시도들을 통해 다가올 미래를 준비한다면, 보다 나은 성과를 이룰 수 있는 기회를 만들 수 있을 것이라 판단한다.

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장소: 일산KINTEX
발표코드: **MEDI-2**
발표분야: Current Trend and Future in Metabolic Disease
발표종류: 심포지엄, 발표일시: 목 14:00, 좌장: 이광호

Role of Pyruvate Dehydrogenase in Diabetes and Obesity

이인규

경북대학교 의과대학

Pyruvate is a critical intermediate in the glucose oxidation and an important precursor for the synthesis of glucose, glycerol, fatty acids, and non-essential amino acids. The regulatory mechanisms for its metabolism are becoming more important. The pyruvate dehydrogenase kinases (PDKs) regulate pyruvate oxidation by controlling the activity of the pyruvate dehydrogenase complex (PDC). The physiological importance of regulation of PDC activity by PDK isoenzyme 2 was assessed by comparing PDK2 knockout (PDK2 KO) mice with wild type mice fed a high fat diet (HFD) and an isocaloric low fat diet (LFD). Body weight gain and hepatic steatosis were attenuated by PDK2 deficiency in the HFD fed mice. Fasting blood glucose, serum insulin, and liver pyruvate, lactate, oxaloacetate, citrate, diacylglycerols, and triacylglycerols were also reduced. Hepatic glucose production was also reduced and insulin sensitivity was increased in the HFD-fed PDK2 KO mice. The hepatic enzyme capacity for fatty acid oxidation and ketogenesis was increased while the capacity for lipogenesis was decreased. In spite of this but consistent with greater PDC activity, the respiratory exchange ratio was higher in the PDK2 knockout mice. Energy expenditure was increased without a difference in physical activity. Increased hepatic insulin sensitivity and improved glucose tolerance correlated with reduced PKCε phosphorylation. The findings support the premise that PDK2 is a potential therapeutic target for hepatic steatosis and insulin resistance.

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발표코드: **MEDI-3**
발표분야: Current Trend and Future in Metabolic Disease
발표종류: 심포지엄, 발표일시: 목 14:30, 좌장: 이광호

New Target in Obesity : TAZ modulator and FGF 21

이관우

아주대학교 의과대학 내분비대사내과

서구화된 식습관과 운동부족으로 인하여 비만, 당뇨병과 같은 대사 질환 환자가 급속하게증가하고 있다. 따라서 비만과 당뇨병을 예방하고 치료하기 위한 연구가 다방면에서 진행되고 있다. 최근연구에서는 14-3-3 결합 단백질인 TAZ (transcriptional co-activator with PDZ-binding motif)가 지방세포분화를 유도하는 PPAR-gamma 를 억제함이 보고되었고, Mitokine 인 fibroblast growth factor 21(FGF21)이 lipolysis, fatty acid oxidation 과 white adipose tissue 의 browning 을 증가시켜 비만 및 당뇨병을 개선시킨다는 보고가 있어서 비만환자에서의 새로운 치료제로서의 중요성이 부각되고 있다. 이에 연자는 비만과 당뇨병에서 TAZ 와 FGF21 이 미치는 영향을 살펴보고자 한다. 생쥐 근육세포인 C2 myotubes 와 C57BL/6J 생쥐에서 고농도 지방산 및 고지방식이에 의한 염증신호(TNF-alpha, IL-1beta, IL-6 and MCP-1)와 인슐린신호(AKT, Glucose uptake)의 변화를 확인하고, 최근 화학연구원에서 확인한 TAZ modulator(activator), TM-25659 에 의해 어떻게 조절되는지 관찰하였다. C2 myotubes 에서 pamitate 를 처리했을때 p-AKT 와 Glucose uptkae 가 감소하고, pro-inflammation cytokine 인 TNF-alpha, IL-1beta, IL-6 and MCP-1 이 증가하였으나, 이러한 현상은 TAZ modulator 인 TM-25659 에 의해 모두 회복됨을 보였다. 당뇨환자군이 정상대조군에 비해 혈중 FGF21 농도가 증가되어있는 것을 확인하였으며, 당뇨환자군내에서는 carotid artery plaque 가 있는 환자의 혈중 FGF21 농도가 carotid artery plaque 가 없는 환자 보다 더 높은 것을 확인하였다. 또한, Human skeletal muscle myotubes 에서 고농도 지방산에 의한 인슐린저항성 모델에서 FGF21 투여로서 인슐린저항성이 회복됨을 확인하였고, 이는 stress kinase 와 NF-κB 의 억제를 통하여짐을 증명하였다. 결론적으로, FGF21 과 TAZ modulator 가 당뇨병과 비만에서 일어나는 염증과 인슐린저항성 개선효과에 기여할 수 있음을 논고(論告)하고자한다.

일시: 2014년 4월 16~18일(수~금) 3일간
장소: 일산KINTEX
발표코드: **MEDI-4**
발표분야: Current Trend and Future in Metabolic Disease
발표종류: 심포지엄, 발표일시: 목 15:00, 좌장: 곽영신

대사질환 동물모델 및 당뇨비만 연구

이상달

한국화학연구원 약리활성연구그룹

당뇨병은 풍요로운 식생활이 가능해진 현대에 있어 사람의 건강을 크게 위협하는 질병이다. 산업화가 급격히 진행되면서 당뇨병 발병률도 함께 빠르게 증가하고 있는데 특히 비만의 증가와 밀접한 연관이 깊다. 당뇨병은 발병에 영향을 미치는 유전자의 수가 많은 전형적인 다유전자형(polygenic) 질병이다. 이에 활동이 부족한 생활습관과 고지방 음식 등의 환경요인이 결합하면서 발병하는데, 다양한 원인에 의한 비만과 이에 따른 인슐린저항성의 발생이 당뇨병의 발병의 원인으로 지목된다. 복잡한 당뇨병의 발병특징으로 인하여 사람에서 원인이 되는 유전자와 환경에 대한 연구를 하는 것이 쉽지 않기 때문에 질환모델동물을 이용한 연구가 많이 진행되고 있다. 특히 마우스와 랫드를 포함하는 설치류가 많이 사용되는데, 이는 설치류의 당뇨병 발병기전이 사람의 그것과 완전히 일치하지는 않지만 사람과 설치류의 당뇨병 양상이나 치료제에 대한 반응이 다른 질병에 비하여 비교적 높은 상관관계를 가지고 있기 때문이다. 마우스의 경우 연구의 필요성에 의하여 근교계(inbred strain)로 유지되는 경우가 많은데 특정한 근교계 내에서 유전적으로 높은 동질성을 가지고 있다. 각 근교계들의 유전적인 배경이 많은 차이가 나기 때문에 근교계에 따라서 비만이나 당뇨병을 발현시키는 다양한 환경 또는 처치에 대한 반응이 전혀 다르게 나타난다. 그러므로 당뇨병이나 비만의 발병 원인연구나 치료제 개발연구에서는 각 계통의 특징을 제대로 알고 연구목적에 알맞은 계통을 사용해야한다. 또한 현재 개발되어 있는 동물들은 근교계의 특성상 사람들의 다양한 질병특성을 반영할 수 없다는 것도 알고 있어야한다.

일시: 2014년 4월 16~18일(수~금) 3일간

장소: 일산KINTEX

발표코드: **MEDI-5**

발표분야: Current Trend and Future in Metabolic Disease

발표종류: 심포지엄, 발표일시: 목 15:30, 좌장: 곽영신

Business consideration in diabetes research

신현우

보건산업진흥원 제약산업 지원팀

Due to the exploding increase in the number of diabetes patients along with world economic growth and increase of life expectancy, diabetes became a major research focus among big pharmaceutical companies, research institutes, and academia for past years.As a result, diabetes research area became heavily competitve by many pipelines in the development and profitability was challenged by many generic drugs. In this presentation, some business concern will be presented including competitve landscape, price information associated with formulary, licensing history and development strategy

일시: 2014년 4월 16~18일(수~금) 3일간
장소: 일산KINTEX
발표코드: **MAT1-1**
발표분야: Two-Dimensional Materials: Graphene, Transition Metal Dichalcogenides, and Others I
발표종류: 심포지엄, 발표일시: 목 09:10, 좌장: 신현석

New Carbon Materials

Rodney Scott Ruoff

[1]Center for Multidimensional Carbon Materials (CMCM), Institute for Basic Science (IBS) [2]Department of Chemistry, Ulsan National Institute of Science and Technology (UNIST)

We discuss a variety of new carbon materials including new allotropes of carbon that are important targets for synthesis. If these new carbon materials can be made, their exceptional properties will herald new discoveries in physics and other areas of science, and they will find use in a wide range of important applications. They offer exciting challenges for understanding chemical reaction pathways and for achieving fine control over the spatial distribution of trivalent and tetravalently bonded carbon. Related materials with boron and nitrogen and other elements are of parallel interest.

일시: 2014년 4월 16~18일(수~금) 3일간
장소: 일산KINTEX
발표코드: **MAT1-2**
발표분야: Two-Dimensional Materials: Graphene, Transition Metal Dichalcogenides, and Others I
발표종류: 심포지엄, 발표일시: 목 09:40, 좌장: 신현석

Interesting Properties of Strained and Defective Graphene

Kian Ping Loh

Department of Chemistry and Graphene Research Centre, National Univeristy of Singapore, Singapore

Most people think of graphene as a flat membrane and the quality of physics observation depends on the flatness of it. However defective or strained graphene can present interesting properties, especially to a chemist. For example, generating pores or voids in graphene, oxidizing and disrupting the conjugation, as in the case of nanoporous graphene oxide, can generate a material that is catalytically active ? what the chemists called “carbocatalyst”. Nanoporous graphene oxide can mediate a wide range of chemical transformation. We have managed to identify a simple chemical treatment to introduce porosity and tune the acidity of Graphene Oxide (GO). This is a potentially important area for industrial applications [1]. The GO catalyst can be used in oxidative coupling reactions as well as tandem catalytic reactions.

Generating strain textures on graphene allows the engineering of new energy landscape. The Dirac electrons in graphene couples to strain via pseudomagnetic field, creating an electrodynamics that is controlled by the geometry of the strain. Using the graphene Moir? superlattice, geometrically precise nanobubbles can be generated that show pseudomagnetic field in the hundreds of Telsa [2]. We discuss the chemistry of how such strain texture can be created by controlling sub-surface defects on the metal substrate. Nanobubbles on graphene can also be created when graphene is transferred onto diamond. Very robust interfacial bonding between diamond and graphene allows a hydrothermal anvil to be created at the interface. Superheated water trapped at the interface becomes corrosive at high temperature and pressure and can etch diamond [3]. By monitoring the conformational changes of pressure-sensitive molecules , the pressure within the nanobubble could be tracked as a function of temperature and was found to be at ~1 GPa at 600 deg C. The polymerization of buckminsterfullerene(C60), which is symmetrically forbidden under ambient conditions, was observed to proceed in well-defined stages in the pressurized nanobubbles.

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장소: 일산KINTEX

발표코드: **MAT1-3**

발표분야: Two-Dimensional Materials: Graphene, Transition Metal Dichalcogenides, and Others I

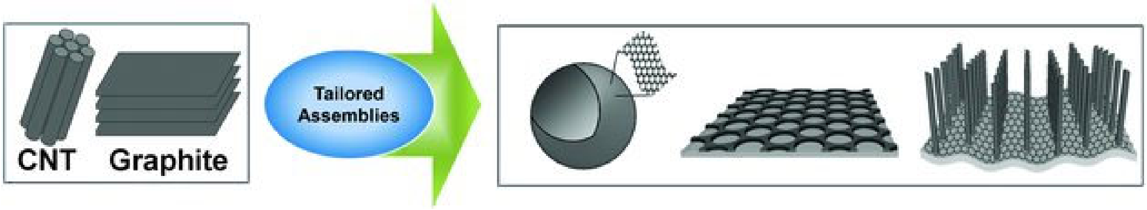
발표종류: 심포지엄, 발표일시: 목 10:10, 좌장: 신현석

Nanoscale Assembly & Chemical Modification of Carbon Nanotubes and Graphene for Nanomaterials & Nanodevices

김상욱

한국과학기술원(KAIST) 신소재공학과

Graphitic carbon nanomaterials, including fullerene, carbon nanotubes and graphene, attract enormous research attention for their outstanding material properties along with molecular scale dimension. The optimized utilization of those graphitic carbons in various application fields inevitably requires the subtle controllability of their structures and properties. In this presentation, our recent research achievements associated to nanoscale molecular scale assembly and chemical modification of graphitic carbon nanomaterials will be presented. Graphitic carbons can be efficiently processed into various three-dimensional structures employing self-assembly principles. Those carbon assembled structures with extremely large surface and high electro-conductivity are potentially useful for catalysis, energy storage and so on. In addition, the substitutional doping of graphitic carbon with B- or N- was achieved via pre- or post-synthetic treatment. The resultant chemically modified graphitic carbons with tunable workfunction and remarkably enhanced surface activity could be employed for organic solar cells, organic light emitting diodes, supercapacitors, Li-ion batteries, nanocomposites, nanocatalysts with improved functionalities and devices performances.



일시: 2014년 4월 16~18일(수~금) 3일간

장소: 일산KINTEX

발표코드: **MAT1-4**

발표분야: Two-Dimensional Materials: Graphene, Transition Metal Dichalcogenides, and Others I

발표종류: 심포지엄, 발표일시: 목 11:00, 좌장: 류순민

2D nanosheets of inorganic solids: inorganic analogues of graphene with tailorable properties and functionalities

황성주

이화여자대학교 화학·나노과학과

Over the past decade, my group has carried out systematic study on the exploration of 3D heterostructured hybrid materials with diverse functionalities using the exfoliated 2D nanosheets of layered inorganic solids (layered metal oxides, layered double hydroxides, layered metal chalcogenides, and graphene). Main purpose of our researches is to explore novel functional materials applicable for energy and environmental technologies. The 2D nanosheets of inorganic solids and graphene can be used as efficient precursors for porous heterostructured nanohybrids, multilayered films, porous hollow spheres, layer-by-layer-deposited (LbL) films, etc. I will present several practical examples of the 2D inorganic/graphene nanosheets and their nanohybrids with tailorable physicochemical properties and functionalities such as electrochemical activity, photocatalytic activity, redox catalytic activity, electrocatalytic activity, gas adsorption capability, and nanobio application.

일시: 2014년 4월 16~18일(수~금) 3일간

장소: 일산KINTEX

발표코드: **MAT1-5**

발표분야: Two-Dimensional Materials: Graphene, Transition Metal Dichalcogenides, and Others I

발표종류: 심포지엄, 발표일시: 목 11:30, 좌장: 류순민

Edge-Selectively Functionalized Graphene Nanoplatelets as Efficient Electrocatalysts

백종범

울산과학기술대학교(UNIST) 에너지공학부

The scalable production of heteroatom-doped graphene nanoplatelets (GnPs) is an important challenge for many applications in practice. Here, we demonstrate efficient and eco-friendly methods for the large-scale synthesis of low-cost and high-quality GnPs and their applications. The approach involves edge-selective functionalization of graphite as a precursor for GnPs via a “direct” covalent attachment of organic molecular wedges and/or functional groups to the edges of pristine graphite. It is an important step toward high-yield exfoliation of three-dimensional graphite into two-dimensional GnPs with minimal basal plane distortion. The resultant edge-selectively functionalized GnPs (EFGnPs) displayed outstanding electrocatalytic activity. Our findings suggest that the EFGnPs can be prepared and conveniently used as base materials for a wide range of applications from wet chemistry to device applications.

일시: 2014년 4월 16~18일(수~금) 3일간

장소: 일산KINTEX

발표코드: **MAT2-1**

발표분야: Two-Dimensional Materials: Graphene, Transition Metal Dichalcogenides, and Others II

발표종류: 심포지엄, 발표일시: 목 13:30, 좌장: 백종범

Chemistry in Two-Dimension

홍병희

서울대학교 화학부

Graphene has unique mechanical, electronic, and optical properties, which researchers have used to develop novel electronic materials including transparent conductors and ultrafast transistors. Recently, the understanding of various chemical properties of graphene has facilitated its application in high-performance devices that generate and store energy. Graphene is now expanding its territory beyond electronic and chemical applications toward biomedical applications. In this talk, recent advances in graphene-related chemistry will be reviewed first, and novel chemical phenomena in 2-dimension enabled by the unique properties of graphene will be reported, including graphene catalyzed/inhibited reactions, *in-situ* observation of 2D liquids in graphene liquid cell, unusual optical and chemical behaviors of molecules between graphene layers, etc.

일시: 2014년 4월 16~18일(수~금) 3일간

장소: 일산KINTEX

발표코드: **MAT2-2**

발표분야: Two-Dimensional Materials: Graphene, Transition Metal Dichalcogenides, and Others II

발표종류: 심포지엄, 발표일시: 목 14:00, 좌장: 백종범

New opportunities in transferred CVD graphene

Lay-Lay CHUA

Departments of Chemistry and Department of Physics, National University of Singapore, Singapore

In this talk, I would describe some new applications opened up by soft transfer method that can transfer graphenes to almost all surfaces, including polymer thin films and hydrophobic surfaces. The transfer method is based on the development of a non-adhesive self-release layer (SRL) used together with a conventional poly(dimethylsiloxane) elastomer stamp with pick-and-place capability. This novel transfer methodology is also applicable to other 2D materials. We demonstrate graphene as electrodes, buffer layers and charge-injection layers. We also describe the use of this method to transfer other thin materials films.

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장소: 일산KINTEX
발표코드: **MAT2-3**
발표분야: Two-Dimensional Materials: Graphene, Transition Metal Dichalcogenides, and Others II
발표종류: 심포지엄, 발표일시: 목 14:50, 좌장: Rodney Scott Ruoff

Large-Area Synthesis of Hexagonal Boron Nitride and Graphene for Novel Energy Harvesters

김상우

성균관대학교 신소재공학부

Hexagonal boron nitride (h-BN) has received a great deal of attention as a substrate material for high-performance graphene electronics, because it has an atomically smooth surface, lattice constant similar to that of graphene, large optical phonon modes, and a large electrical band gap. I will present the large-scale synthesis of high-quality h-BN nanosheets in a chemical vapor deposition (CVD) process by controlling the surface morphologies of the copper (Cu) catalysts. It was found that morphology control of the Cu foil is much critical for the formation of the pure h-BN nanosheets as well as the improvement of their crystallinity. We demonstrate the performance enhancement of CVD-based graphene devices with large-scale h-BN nanosheets. The mobility of the graphene device on the h-BN nanosheets was increased three times compared to that without the h-BN nanosheets. The on-off ratio of the drain current is two times higher than that of the graphene device without h-BN. This work suggests that high-quality h-BN nanosheets based on CVD are very promising for high-performance large-area graphene electronics.

As a second issue, I will address graphene-based novel energy harvesters. The rapid development of graphene has increased the demand for next generation electronics. The application of graphene as an exciting transparent and flexible mechanical energy scavenging device is an effective approach for sustainable and green power source for wireless, portable and implanted electronics. We experimentally demonstrate the first application of CVD grown graphene as an energy-generating active material for transparent flexible triboelectric nanogenerator (NG) and its high electric output power generation under vertical compressive strain. NGs based on mono, double, triple, quadruple and few layers of graphene (grown on Cu-foil and Ni-foil via CVD approach) have been fabricated and their output voltage and current were measured under mechanical strains. Monolayer based graphene NG exhibits high power compared to other randomly staked graphene layer based NG, while output voltage and current from conventional staked few layers based NG (grown on Ni-foil via CVD approach) reached up to maximum value of 9.0 V and 1.2 $\mu A/cm^2$, with conversion efficiency up to 8.7 %. This study provides a facile new avenue for harvesting mechanical energy from transparent flexible graphene based NG for self-powered systems.

일시: 2014년 4월 16~18일(수~금) 3일간

장소: 일산KINTEX

발표코드: **MAT2-4**

발표분야: Two-Dimensional Materials: Graphene, Transition Metal Dichalcogenides, and Others II

발표종류: 심포지엄, 발표일시: 목 15:20, 좌장: Rodney Scott Ruoff

Unique properties of semiconducting two-dimensional crystals

Goki Eda

Department of Physics/Chemistry, National University of Singapore Graphene Research Centre, National University of Singapore

Semiconducting two-dimensional (2D) crystals derived from layered transition metal dichalcogenides (TMD) are attractive building blocks for novel electronic and optoelectronic devices [1,2]. In this talk, I will discuss the electronic properties of group 6 TMD 2D crystals based on charge transport and photoluminescence (PL) spectroscopy studies.

A single layer MoS2 is a direct gap semiconductor in striking contrast to its indirect gap bulk counterpart [3]. As a result, single layer MoS2 exhibits distinct band gap PL. We have shown that mono- to few-layer WS2 and WSe2 that their band structure undergoes the same indirect-to-direct gap transition at the limit of a single monolayer [4]. Based on temperature-dependent PL spectroscopy, we further reveal subtle but fundamental differences in the conduction band structure of few-layer MoS2, WS2, and WSe2. Specifically, the effect of thermally modulated band structure on the recombination of indirect excitons will be discussed [5]. We further demonstrate using PL excitation spectroscopy that band nesting has a unique effect on the relaxation pathway of photoexcited carriers.

I will also discuss about the recent success in the growth of monolayer TMDs via chemical vapor deposition (CVD) and our recent findings on the electronic quality of CVD MoS2 monolayer thin films through charge transport studies. I will discuss our current understanding on the factors limiting carrier mobility in these materials.

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일시: 2014년 4월 16~18일(수~금) 3일간

장소: 일산KINTEX

발표코드: **MAT2-5**

발표분야: Two-Dimensional Materials: Graphene, Transition Metal Dichalcogenides, and Others II

발표종류: 심포지엄, 발표일시: 목 15:50, 좌장: Rodney Scott Ruoff

Raman Metrology for Graphene and its Application in Surface Scientific Problems

류순민

경희대학교 응용화학과

Raman spectroscopy has proven to be a versatile analytical tool in graphene research because of the varying spectral features for different thickness, stacking, defect density, charge density (n), mechanical strain (ε), temperature, etc. Such multimodal sensitivity, however, turns into difficulty when multiple unknown variables are to be determined simultaneously. Despite the strain-sensitivity of the Raman G and 2D modes, for example, optical characterization of native strain in graphene on silica substrates has been hampered by excess charges interfering with both modes. In this talk, I will show that the effects of strain and charges in graphene can be optically separated from each other by correlation analysis of the two modes, enabling simple quantification of both.[1] Additionally, the change in the electronic structure of graphene caused by the van der Waals interaction with hexagonal boron nitride (hBN) substrates can also be optically determined.[2] Employing the proposed analysis, I will address our recent findings on important surface scientific issues of graphene such as structural deformation caused by substrates and thermal perturbation,[1] interfacial charge transfer,[3, 4] and molecular intercalation[5] through graphene-substrate interface.

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일시: 2014년 4월 16~18일(수~금) 3일간
장소: 일산KINTEX
발표코드: **ELEC1-1**
발표분야: Electrochemistry on New Electrode Materials I
발표종류: 심포지엄, 발표일시: 목 09:20, 좌장: 김규원

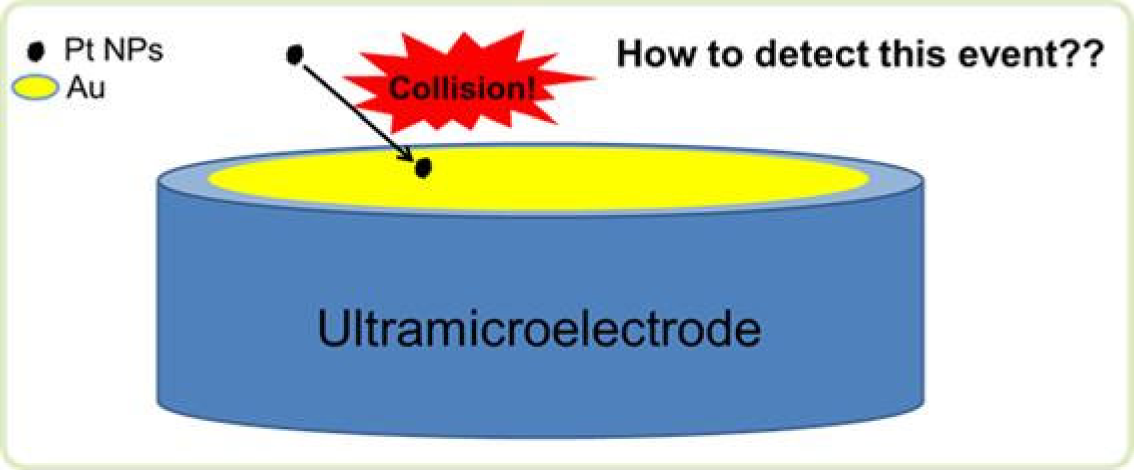
Electrochemical detection of a single nanoparticle in aqueous solution

박준희

전북대학교 화학교육과

나노과학은 현대과학을 이끌고 있는 큰 흐름으로 현재 석유화학에서부터 생활가전에 이르기까지 널리 응용되고 있으며 현대인의 삶에 커다란 혜택을 주고 있다. 미래 산업으로 대변되는 에너지산업을 풀어갈 열쇠는 나노촉매과학이 쥐고 있다고 여겨지며, 현재 학계 및 산업에서 활발한 연구가 진행되고 있다. 나노과학은 나노입자의 크기 효과(size effect)가 발견된 이래로 활발한 연구가 시작되었다. 1 단계의 나노입자 연구는 나노입자의 크기 조절에 따른 그 특성변화에 주목하였으나, 현재는 나노입자의 표면구조 (surface orientation), 격자구조, 산화수, 합금 조절에 따른 촉매성 변화에 대한 연구가 많이 진행되고 있다. 하지만 현재까지의 나노입자의 촉매성 연구는 나노입자 앙상블(ensemble)의 평균 특성을 확인하는 방식으로 진행되어왔다. 일반적 나노입자의 합성 단위인 단위부피(mL)당 약 10^9~10^{12} 개가 넘는 많은 입자들을 완벽히 균일하게 제조 하는 것이 불가능하기 때문에, 이 방식의 연구는 나노입자의 촉매특성을 연구함에 있어 제한 점이었다. 궁극적으로, 단일입자 하나만을 선택적으로 채집해서 연구할 수 있다면 나노입자 연구의 새로운 지평을 열 수 있을 것이다. 현재 단일 나노입자 연구에 대한 노력의 일환으로 단일 나노입자가 전극에 충돌하는 현상을 관찰하는 방법에 대한 연구가 몇 개의 연구단에서 활발히 보고되고 있다. 단일 나노입자 검출법은 여러 가지 측면에서도 중요성을 지닌다. 단 하나의 입자를 검출할 수 있다는 것은 zepto (10^{-21}) molar detection 과 그 궤를 같이한다고 할 수 있다. 용액 속에 단 하나입자만 있어도 검출기와 만나기만 하면 검출 할 수 있기 때문에 고감도 검출을 목표로 하는 바이오센서 연구자에게도 흥미로운 주제일 것이다. 또한 단일 나노입자에서 더 발달시켜 용액상에서 단일 분자를 검출 하는 것은 분석화학 연구자들의 오랜 염원이기도 하다. 따라서 본 발표에서는 단일 입자를 전기화학을 이용해 검출하는 방법을 소개하고자 한다. 전기화학적 활성을 띈 구형 나노입자가 하나가 전기화학적 활성을 띄지 않는 마이크론 크기의 미세 전극에 충돌 후 흡착된다면 비활성인 무한한 평면 위에 놓인 하나의

구 나노전극과 같은 거동을 보일 것이다. 나노 전극은 빠른 시간 내에 정상 상태(steady state)에 이르게 되고 그 크기에 따라 한계전류(steady state limiting current)값을 가지게 된다. 따라서 나노입자가 하나씩 순차적으로 미세전극에 붙게 된다면 시간에 따라 계단형으로 증가하는 전류곡선을 얻을 수 있을 것이다.



일시: 2014년 4월 16~18일(수~금) 3일간
장소: 일산KINTEX
발표코드: **ELEC1-2**
발표분야: Electrochemistry on New Electrode Materials I
발표종류: 심포지엄, 발표일시: 목 10:00, 좌장: 김규원

Quantum-Sized Metal Nanoclusters: A New Electrode Material for Electrochemical Sensing

이동일

연세대학교 화학과

Research on the chemistry and electrochemistry of atomically precise gold nanoclusters, for example, Au25, Au38, Au67, Au102 and Au144, has been extensively pursued in recent years. These nanoclusters exhibit novel electronic, optical and catalytic properties that differ substantially from the corresponding atoms or bulk materials. This presentation reports electrochemical and optical properties of these nanoclusters and their use in electrochemical sensing. Voltammetry of these nanoclusters exhibited well-resolved, reversible redox peaks and size-dependent electrochemical HOMO-LUMO gaps that could be correlated to optical and calculated energy gaps. These nanoclusters also showed excellent electrocatalytic activity toward oxidation of biologically relevant analytes. The modified electrode film prepared with Au25 nanoclusters exhibited excellent mediated electrocatalytic activity that was utilized for amperometric sensing of dopamine and glucose. The electron transfer dynamics in the Au25 film was examined as a function of Au25 concentration, which manifested the dual role of Au25 as an electronic conductor as well as a redox mediator. The electron transfer study has further revealed the correlation between the electronic conductivity of the Au25 film and the sensing sensitivity.

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발표코드: **ELEC1-3**

발표분야: Electrochemistry on New Electrode Materials I

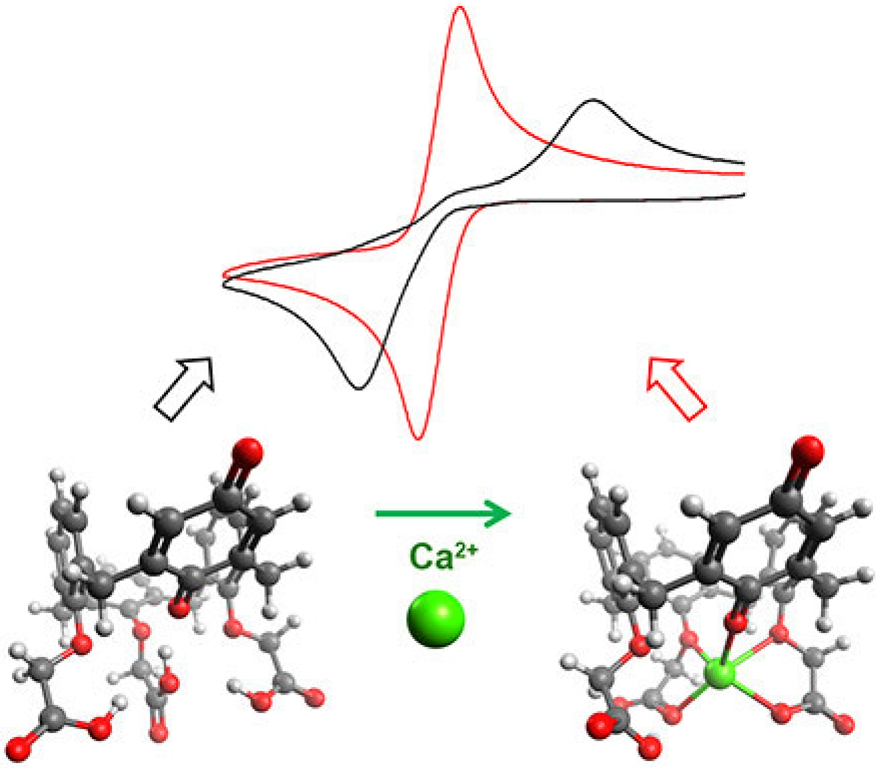
발표종류: 심포지엄, 발표일시: 목 10:50, 좌장: 이동일

Switching PCET reaction by Ca2+ ion Captured by Calix[4]quinone in Aqueous Media

정택동

서울대학교 화학부

Quinone electrochemistry is one of the classical themes that still remain unclear, particularly, in terms of proton-coupled electron transfer (PCET). Calix[4]arene-triacid-monoquinone (CTAQ), a quinone-containing water-soluble ionophore, was utilized to investigate how PCET reactions of quinones were influenced by redox-inactive metal ions in aqueous environment. This ionophoric quinone deraviative captured a Ca2+ ion that drastically altered the voltammetric behavior of quinone, showing characteristic response to pH and unique redox wave separation. Spectroelectrochemistry verified significant stabilization of the semiquinone, and electrocatalytic currents were observed in the presence of Ca2+-free CTAQ. Using digital simulation of cyclic voltammograms to clarify how the thermodynamic properties of quinones were altered, a simple scheme was proposed that successfully accounted for all the observations. The change induced by Ca2+ complexation was explained on the basis of the combined effects of electrostatic influence of captured metal ion and hydrogen bonding of water molecules with the support of DFT calculation.


Ca^{2+}

일시: 2014년 4월 16~18일(수~금) 3일간
장소: 일산KINTEX
발표코드: **ELEC1-4**
발표분야: Electrochemistry on New Electrode Materials I
발표종류: 심포지엄, 발표일시: 목 11:30, 좌장: 이동일

Use of Indium-Tin Oxide Electrodes for Obtaining Sensitive and Reproducible Electrochemical Sensors

양해식

부산대학교 화학과

지금까지 상용화된 전기화학 센서의 작업전극으로 탄소 전극이나 금 전극이 많이 이용되어 왔다. 하지만, 이러한 전극은 배경전류가 크고 시간에 따른 전기화학 촉매 특성의 변화가 크기때문에 낮은 검출한계를 얻거나 재현성있는 센서 결과를 얻는 데에 한계가 있어 왔다. Indium-Tin Oxide (ITO) 전극은 상대적으로 상용화된 전기화학 센서에 거의 사용되고 있지는 않지만, 최근에 ITO 전극의 낮고 재현성 있는 배경전류 특성을 이용한 고감도 전기화학 센서가 활발히 연구되고 있다. 본 발표에서는 지금까지 ITO 전극을 바이오센서에 응용하기 위해서 개발한 “생체분자를 고정화시키는 방법”, “전기화학 촉매 특성을 변화시키는 방법”, “전기화학적으로 신호를 증폭하는 방법” 등을 소개하고자 한다.

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장소: 일산KINTEX

발표코드: **ELEC2-1**

발표분야: Electrochemistry on New Electrode Materials II

발표종류: 심포지엄, 발표일시: 목 13:30, 좌장: 김종원

Materials Design for Rechargeable Lithium-Air Batteries: Challenges and Progress

이종원

한국에너지기술연구원 신재생에너지연구본부

Rechargeable lithium-air batteries have higher theoretical energy density than state-of-the-art lithium-ion batteries. If successfully developed, they could enable electric vehicles with driving ranges similar to those of gasoline-powered vehicles. During discharge, a Li-air battery generates electricity through an oxidation reaction of a Li anode, and a reduction reaction of oxygen (O_2) on a porous cathode. The reverse reactions occur upon charge. There are still significant challenges that should be overcome to realize this technology. In particular, great challenges exist in air electrodes (cathodes) and electrolytes that determine the capacity, energy efficiency, rate-capability and cyclability. This talk introduces the technical challenges facing development of Li-air batteries with specific attention to electrochemistry and materials, and then presents promising strategies (developed at KIER) to design electrodes and electrolytes that could improve the oxygen reaction kinetics and mitigate the interactions between the electrode and electrolyte.

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발표분야: Electrochemistry on New Electrode Materials II
발표종류: 심포지엄, 발표일시: 목 14:05, 좌장: 김종원

Novel Electrical and Photoelectronic Materials Comprising Reduced Graphene and Conducting Polymers

홍종달

인천대학교 화학과

Since last 20 years, nanostructured multilayered materials based on layer-by-layer (LBL) self-assembly method have been devoted to the creation of their novel functions for a broad range of applications. The LBL-assembly allows the excellent control of film thickness and roughness in a nano-scale by adjusting the charge reversal mechanism and interpenetrations. The presentation outlines our recent activities in the development of novel electrical and optoelectronic materials composed of reduced graphene oxide (RGO) and conducting polymers based on LBL-assembly approach; the first example is the fabrication of a temperature-sensitive PET substrate with the two electron-rich layer components including poly(p-phenylene vinylene) (PPV) and RGO layers. The PET sheets coated with (PPV/RGO)15 films exhibited a photocurrent of 115 μA at an illumination intensity of 1.1 mW and a photoresponsivity of 111.1 mAW?1 at an illumination intensity of 0.5 mW; these are among the best values yet achieved in carbon-based materials. Meanwhile, A multilayer film electrode composed of polyaniline (PANi)/RGO bilayers yielded the excellent capacitive performance in supercapacitor; a volumetric capacitance of 584 F/cm3 at a current density of 3.0 A/cm3 for (PANi/RGO)15 film electrode. This volumetric capacitance is one of the best yet reported for the other carbon-based materials. These intriguing features of the MF-electrodes composed of PANi/RGO multilayer films will contribute to new design of high energy storage devices, especially in a micro-dimension, in order to meet the trend of being lightweight and the small form factor of portable electronic devices.

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발표분야: Electrochemistry on New Electrode Materials II
발표종류: 심포지엄, 발표일시: 목 14:50, 좌장: 황성필

Transmission line equivalent circuit models for solid state electrochemistry

이종숙

전남대학교 신소재공학부

Transmission line models have been usually used for the rough or porous electrodes in liquid chemistry. In this presentation two applications of the transmission line models in solid state electrochemistry will be presented. The status-of-the-art high-temperature solid oxide fuel cells are consisted of the porous Ni-YSZ cermet in hydrogen gas and LSM cathode in oxygen gas separated by a YSZ solid electrolyte membrane. The electrode reaction polarization of these gas electrodes exhibits a Butler-Volmer type relation due to the Nernst-type variation in the gas activities. The gas electrode reaction can be described by the transmission line model with longitudinal resistors, and transverse resistors and capacitors. The parameters can be related to the surface diffusivity and surface (adsorption/desorption) reaction in the gas electrodes. Secondly, the transmission line model can be applied to mixed-ionic-and electronic conductors. Two resistor rails representing the ionic and electronic conduction are connected by the chemical capacitance due to the charge neutrality condition. The transmission line model can be thus applied to evaluate the partial conductivities and chemical diffusivities e.g. of the cathode materials in the lithium batteries, which determines the charge/discharge kinetics. A 3D diffusion model and a 1D diffusion model have been applied to the lithium-rich layered nano-composite oxide and lithium iron phosphates in olivine structure, respectively.

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발표코드: **ELEC2-4**

발표분야: Electrochemistry on New Electrode Materials II

발표종류: 심포지엄, 발표일시: 목 15:25, 좌장: 황성필

Energy Harvesting from Carbon Nanomaterials in a Fluid Flow

한창수

고려대학교 기계공학부

흐르는 이온유체안에서 탄소나노튜브로부터 전압을 발생시킬 수 있다는 이론적 제안과 실험적 선행연구가 2000 년대 초에 이루었졌다. 그 이래로 다양한 연구가 진행되어왔으며, 특히 단일벽 및 다중벽 탄소나노튜브에서 수십 mV 이상의 전압을 발생시키는 결과들이 발표되었다. 또한 유사한 탄소결정물질인 그래핀에서도 마찬가지로 흐르는 이온유체안에서 전압발생의 가능하다는 결과가 발표되었지만, 곧이어 이 전압발생이 그래핀이 아니라 그래핀과 전극사이의 접촉부분에서의 전기화학적특성으로 인한 것임을 주장하기도 하였다.본 발표에서는 기존에 제안된 여러가지 에너지 수확 모델에 대해 검증실험을 통해 원인을 보다 엄밀하게 추정하고자 하였으며, 그 결과로 탄소나노튜브에서는 반도체성과 금속성 및 그래핀에서는 극성유체를 이용한 실험을 수행하였고, 수정된 해석 메커니즘을 제안하였다.

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발표코드: **ENVR1-1**
발표분야: Current Topics in Solar Conversion Technology
발표종류: 심포지엄, 발표일시: 목 09:10, 좌장: 박현웅

Molecular Engineering of Low Band Gap Hole Transporting Material for Perovskite Solar Cells

Mohammad Khaja Nazeeruddin

Laboratory of Photonics and Interfaces, Department of Chemistry and Chemical Engineering, Swiss Federal Institute of Technology, Station 6, CH-1015 Lausanne, Switzerland

Thin-film photovoltaics, from the original vacuum-based inorganic devices, to the solution-processed techniques have attracted intensive attention for solar energy conversion into electricity. Recently, organic-inorganic hybrid perovskites thin film photovoltaics came to the limelight because of their high efficiency, low cost and the ease to make these materials solution processable.1-2 Using methyl ammonium lead iodide (CH3NH3PbI3) perovskite as an absorber layer and spiro-OMeTAD as a hole transport material, power conversion efficiencies (PCE) of over 15% were obtained in both mesoporous and planar heterojunction solar cells.2 Here, we present the synthesis and characterization of a low band gap hole transporting material (HTM) based on quinolizino acridine and its application in perovskite solar cells. The quinolizino acridine compound exhibit HOMO at -5.29 eV, which matches well with perovskite HOMO level. The hole mobility of the quinolizino acridine has been measured, which show an effective hole mobility ranging from 3e-5 to 6e-5 cm2V-1s-1 for electric fields ranging a from 10^8 to 10^9 V cm-1. These results place this new hole transporting material in the range of the commonly used spiro-MeOTAD. The functionalized quinolizino acridine compound function as a p-type HTM in CH3NH3PbI3 solar cells, and as well a light harvester in the visible and near IR regions to complement perovskite absorption yielding power conversion efficiency of 13%.

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발표코드: **ENVR1-2**

발표분야: Current Topics in Solar Conversion Technology

발표종류: 심포지엄, 발표일시: 목 09:35, 좌장: 박현웅

Perovskite Solar Cells: New Horizons in Photovoltaics

박남규

성균관대학교 화학공학부

유무기복합 페로브스카이트 태양전지는 높은효율과 값싼재료 및 공정으로 인하여 최근 태양전지 기술의 새로운 지평을 연 신기술로 각광을 받고 있다. 본 발표에서는 고효율 페로브스카이 태양전지 기술에 대하여 소개할 예정이다. ABX3 화학식을 갖는 페로브스카이트에서 A 자리에 메틸암모니움 또는 이와 유사한 이온반경을 갖는 유기물질이 가능하며, B 자리에는 Pb(2+), Sn(2+) 등이 가능하다. 페로브스카이트 필름은 one-step 코팅기술 또는 two-step 코팅기술로 제작가능하다. Two-step 코팅으로 제작된 경우 one-step 보다 더 우수한 특성을 보이는데 이는 페로브스카이트 모폴로지와 관련성이 있다. Two-step 으로 만든 페로브스카이트 태양전지는 평균 16.4% 이며, 최고효율은 16.9%를 얻었다. 이는 현재까지 보고된 효율 중 가장 높은 값에 해당한다. A 자리에 다른 유기양이온을 치환할 경우 밴드갭 변화가 가능하며, 밴드갭이 더 작은 물질을 이용하여 평균 15.6%, 최고 16% 효율을 얻었다.

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발표종류: 심포지엄, 발표일시: 목 10:00, 좌장: 박현웅

New Materials Strategies for Hybrid Electronic Circuitry

Tobin J. Marks

Northwestern University

This lecture focuses on the challenging design, characterization, and realization of new materials for creating unconventional electronic as well as excitonic circuitry. Fabrication methodologies to achieve these goals include high-throughput, large-area printing techniques. Materials design topics to be discussed include: 1) Rationally designed high-mobility p- and n-type organic semiconductors for printed organic CMOS, 2) Polycrystalline and amorphous oxide semiconductors for transparent and mechanically flexible electronics, 3) Self-assembled and printable high-k nanodielectrics enabling ultra-large capacitance, low leakage, high breakdown fields, minimal trapped interfacial charge, and device radiation hardness. 4) Combining these materials sets to fabricate a variety of high-performance thin-film transistor-based circuitry.

일시: 2014년 4월 16~18일(수~금) 3일간

장소: 일산KINTEX

발표코드: **ENVR1-4**

발표분야: Current Topics in Solar Conversion Technology

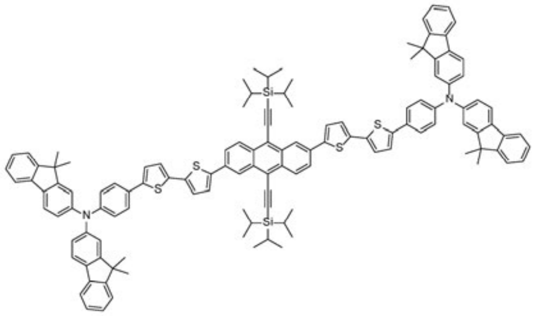
발표종류: 심포지엄, 발표일시: 목 10:40, 좌장: 박현웅

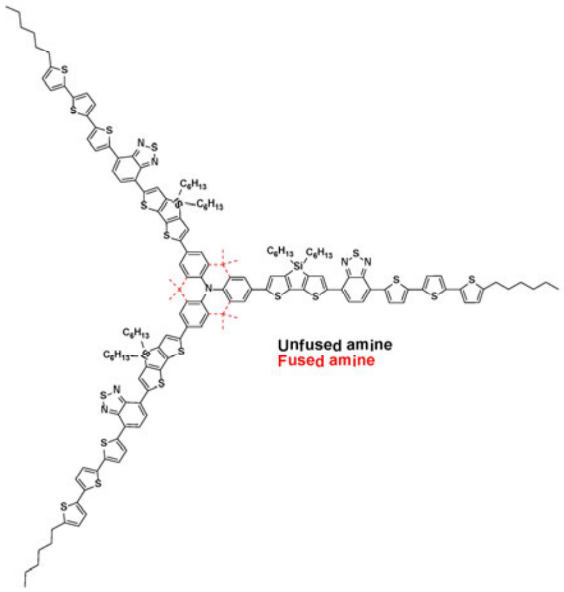
Bulk Heterojunction Organic Solar Cell Using Small Molecules

고재중

고려대학교 소재화학과

Increasing global warming is recognized as the most critical issues encountered in this century. Therefore research target at solar energy harvesting is currently under extensive investigation. One promising technology would be organic solar cell, which is expected to dominate the low-cost market in the future. In the organic solar cell, numerous polymers have been used as light harvest. Due to the synthetic difficulty, molecular weight distribution, many research groups have expended endeavors to develop small molecules as the alternative sensitizers, which are easy to the synthesis. Recently, impressive photovoltaic performances have been reported on various well designed small molecules, showing promising efficiency in the range of 5~8.5%. Recently, we synthesized a new series of small molecules with thiophene perylene bisimide, benzothiadiazole, anthracene based chromophore and planar star-shaped unit. In this presentation, we want to report various different type of small molecules for efficient organic solar cells.


Si
Si
N
N
S


S
N
Si
C_6H_{13}
N
Unfused amine
Fused amine

일시: 2014년 4월 16~18일(수~금) 3일간
장소: 일산KINTEX
발표코드: **ENVR1-5**
발표분야: Current Topics in Solar Conversion Technology
발표종류: 심포지엄, 발표일시: 목 11:05, 좌장: 박현웅

Heterojunctions at Metal Oxide Semiconductors for Solar Photocatalytic and Photosynthetic Applications

최원용

포항공과대학교 환경공학부

The photoinduced electron transfers occurring at the semiconductor surface are the key process of solar photosynthetic and photocatalytic processes. Metal oxides such as TiO2, WO3, and Fe2O3 that consists of earth-abundant elements are the most practical base materials for such applications. Despite their popularity as solar conversion materials, breakthroughs in materials development have yet to be achieved for practical applications. A variety of approaches have been investigated to modify the base metal oxides using diverse inorganic and organic materials. The heterojunctions built at the interface of metal oxide reduce the charge recombination or enhance the interfacial charge transfer to achieve the higher conversion efficiency. In this talk, various modifications of metal oxides with interfacial heterojunctions will be introduced and discussed for photocatalytic and photosynthetic applications. The specific examples include thin alumina layer coated WO3 for water oxidation, thin TaOxNy layer coated N-TiO2 nanotubes for water splitting, TiO2/graphene composites for photocatalysis, and charge transfer complexation on the surface of TiO2. Each modification method has a different effect on the solar conversion activity and the mechanisms, which will be discussed in detail.

일시: 2014년 4월 16~18일(수~금) 3일간

장소: 일산KINTEX

발표코드: **ENVR1-6**

발표분야: Current Topics in Solar Conversion Technology

발표종류: 심포지엄, 발표일시: 목 11:30, 좌장: 박현웅

Powering Ahead with Solar Energy

Lesley Yellowlees

University of Edinburgh

In order to meet the ever increasing demand for electricity from an ever increasing global population it will be necessary to turn to renewable sources. One area where chemists can contribute effectively is in Solar Energy. The lecture will describe Dye Sensitised Solar Cells and the research we have undertaken in Edinburgh to characterise such cells using techniques such as uv/vis and epr spectroelectrochemistry.

일시: 2014년 4월 16~18일(수~금) 3일간

장소: 일산KINTEX

발표코드: **ENVR2-1**

발표분야: Trends in Green Chemistry: Biosynthetic and Biomimetic Technologies

발표종류: 심포지엄, 발표일시: 목 13:00, 좌장: 황동수

Metal-impregnated Biological Materials: Examples and Mimicking

이승모

한국기계연구원 나노역학 연구실

In nature, tiny amounts of inorganic impurities, such as metals, incorporate in protein structures of some biomaterials and lead to unusual mechanical properties of these materials. A desire to produce those bio-mimicking new materials has constantly stimulated material scientists and up to now diverse approaches have been attempted. In contrast, the research to improve the mechanical properties of biomaterials themselves by direct metal incorporation into inner-protein structures of those has been rarely tried due to the difficulty to develop a method which can infiltrate metals into biomaterials, resulting in a metal incorporated protein matrix. In this talk, it will be demonstrated that metals can be intentionally infiltrated into inner protein structures of biomaterials through “Multiple Pulsed Vapor Phase Infiltration” performed in equipment conventionally used for atomic layer deposition (ALD) process. Some examples will be introduced, such as dragline silks from Araneus spider and collagen, which show highly improved toughness after transition metal infiltration. The result on enhanced toughness of spider silk and collagen could potentially serve as a model case for a more general approach to enhance the strength and toughness of other biological or natural matters.

일시: 2014년 4월 16~18일(수~금) 3일간
장소: 일산KINTEX
발표코드: **ENVR2-2**
발표분야: Trends in Green Chemistry: Biosynthetic and Biomimetic Technologies
발표종류: 심포지엄, 발표일시: 목 13:25, 좌장: 황동수

Silica synthesis induced by silk protein - Factors affecting the yield and morphology

이기훈

서울대학교 바이오시스템소재학부

Silkworm produces two kinds of proteins, namely fibroin and sericin. Sericin envelops two brins of fibroin and usually removed during the degumming process in order to achieve softness of textile. In this study, we tried to synthesize silica using sericin by biomimetic method. We have prepared silica directly from its precursor without hydrolysis in the presence of silk sericin, which is similar to silicatein protein found in marine sponges. We only mixed tetraethyl orthosilicate (TEOS) and sericin aqueous solution and left in the laboratory at ambient condition. A white precipitate was formed at the interphase, and the formation of silica was identified by various analyzing techniques. The yield of silica was affected by the type of sericin and pH. Selective blocking of aspartic acid and histidine of sericin reduces the yield of silica significantly indicating important role of these amino acids during silica synthesis. We further found that the secondary structure of sericin can affect the morphology of final silica particle. We expect that sericin could be used as an alternative of silicatein.

일시: 2014년 4월 16~18일(수~금) 3일간

장소: 일산KINTEX

발표코드: **ENVR2-3**

발표분야: Trends in Green Chemistry: Biosynthetic and Biomimetic Technologies

발표종류: 심포지엄, 발표일시: 목 13:50, 좌장: 황동수

Small Molecule Activation by Mimicking Active Sites of Metalloenzymes

조재홍

대구경북과학기술원(DGIST) 신물질과학

Small molecule activation by transition metal centers is essential to numerous stoichiometric and catalytic organic transformations in biological and industrial processes. Nature has gone through a course of trial and error to refine the living creatures, processes, and materials over 3.6 billion years. Oxygen-coordinating metal intermediates, such as metal?superoxo, ?peroxo, ?hydroperoxo, and ?oxo species, are frequently invoked as plausible oxidants in the oxidation of organic substrates in the living organisms. Among the metal?oxygen adducts, metal?superoxo species have attracted much attention recently, since the intermediates have been implicated as reactive species in the C-H bond activation of substrates by nonheme iron (e.g., isopenicillin N synthase and myo-inositol oxygenase) and copper (e.g., dopamine β-monooxygenase and peptidylglycine-α-amidating monooxygenase) enzymes. In this work, we have shown the first structurally characterized end-on chromium(III)-superoxo complex, $[Cr^{III}(O_2)(TMC)(Cl)]^+$ (TMC = 1,4,8,11-tetramethyl-1,4,8,11-tetraazacyclotetradecane), which was synthesized by reacting $[Cr^{II}(TMC)(Cl)]^+$ with O_2. The Cr(III)-superoxo intermediate has shown reactivities in C-H cleavage of alkylaromatics via an H-atom abstraction mechanism. In addition, we report that $[Cr^{III}(O_2)(TMC)(Cl)]^+$ is able to transfer its oxygen atom to organic substrates (e.g., PPh_3 and sulfides), yielding the corresponding oxygenated products and a chromium(IV)?oxo complex, $[Cr^{IV}(O)(TMC)(Cl)]^+$.

일시: 2014년 4월 16~18일(수~금) 3일간
장소: 일산KINTEX
발표코드: **ENVR2-4**
발표분야: Trends in Green Chemistry: Biosynthetic and Biomimetic Technologies
발표종류: 심포지엄, 발표일시: 목 14:15, 좌장: 황동수

Laccase-catalyzed biotransformation of natural phenols for biotechnological applications

장윤석

포항공과대학교 환경공학부

Laccases are one of the promising oxidases for industrial applications due to their versatile reactivity and robustness. In most applications, the enzymatic actions start with single-electron oxidation of small organics followed by formation of the corresponding radicals. These radicals are further involved in oxidative coupling, leading to syntheses of oligomers and adducts. In the synthetic approaches of laccases, use of naturally occurring phenol substrates is of great interest because such reactions fulfill the basic requirement of green chemistry, in that little toxic waste is produced. Natural phenols also serve as key substrates for laccase-catalyzed in vivo biosynthetic processes giving rise to natural organics showing various kinds of physicochemical functionalities. The above observation strongly indicates that the synthetic design of in vitro laccase oxidations involving small phenolics should be guided by the knowledge of laccase-driven in vivo metabolic steps. In this talk, I will discuss the fundamental connection between novel synthetic applications and laccase-related in vivo metabolisms and present my on-going roadmap for R&D based on these eco-friendly enzymatic reactions.

일시: 2014년 4월 16~18일(수~금) 3일간
장소: 일산KINTEX
발표코드: **ENVR2-5**
발표분야: Trends in Green Chemistry: Biosynthetic and Biomimetic Technologies
발표종류: 심포지엄, 발표일시: 목 15:05, 좌장: 장윤석

Biomimetic mineralization approach toward functional optical materials

이규복

한국에너지기술연구원 기후변화연구본부

Natural materials often provide material scientists a source of inspiration in developing advanced materials. Especially biominerals and the formation processes exploit efficient pathways of inorganic-based material synthesis. Despite the formation at ambient conditions by using easily accessible and abundant components in nature only, biominerals often show remarkable functionalities. For example, biomineralized calcitic microlenses, as part of the photoreceptor system in brittlestar, Ophiocoma wendtii, are one striking example for an adapted biomineral system. The microlens system is optimized in shape and crystal orientation to correct for aberration effects. In this talk, the recent work on synthetic calcium carbonate microlens arrays will be presented. The microlens arrays are formed simply based on calcium ion and organic molecules in water and CO2 in air under ambient conditions. To elucidate the formation mechanism as well as optical properties of microlens array, we investigate the structures by various microscopic techniques, micro-beam scanning wide-angle X-ray diffraction and Raman spectroscopic imaging. The results show that CaCO3 microlenses have uniform focal length with good optical transparency as well as unique optical property originated from crystal orientation, which suggests taking advantage of biomineralization approach for the synthesis of advanced optical materials.

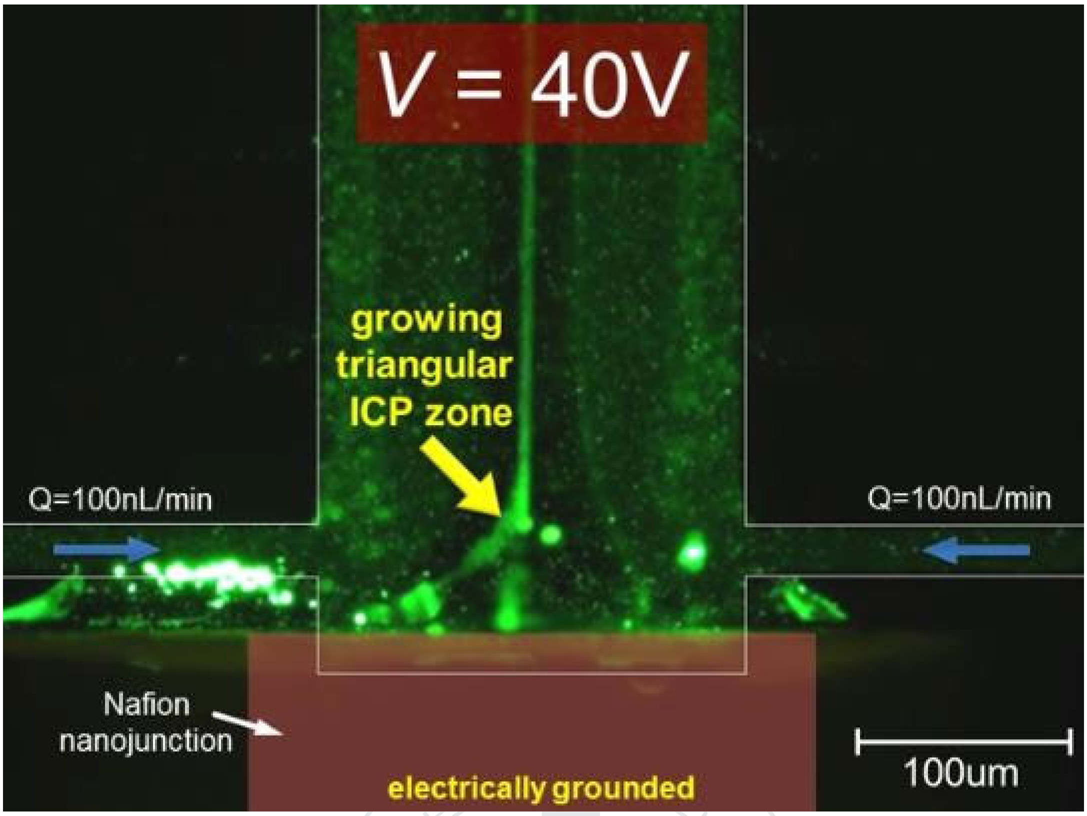
일시: 2014년 4월 16~18일(수~금) 3일간
장소: 일산KINTEX
발표코드: **ENVR2-6**
발표분야: Trends in Green Chemistry: Biosynthetic and Biomimetic Technologies
발표종류: 심포지엄, 발표일시: 목 15:30, 좌장: 장윤석

Nano-electrokinetic and power-free desalination/purification system

김성재

서울대학교 전기정보공학부

Ion Concentration Polarization (ICP) phenomenon is traditional electrochemical ion transportation process and appears as a steep concentration gradient near nanoporous membrane under dc bias. The major function of ICP is an active ion control by an external electric field so that it is significantly useful to study the new ion transportation through nanoporous junction (or membrane) and develop novel engineering applications. As examples, high energy efficient desalination/purification will be introduced and problems behind these applications such as instability will be also discussed.


V = 40V
growing triangular ICP zone
Q=100nL/min
Q=100nL/min
Nafion nanojunction
electrically grounded
100um

일시: 2014년 4월 16~18일(수~금) 3일간
장소: 일산KINTEX
발표코드: **ENVR2-7**
발표분야: Trends in Green Chemistry: Biosynthetic and Biomimetic Technologies
발표종류: 심포지엄, 발표일시: 목 15:55, 좌장: 장윤석

Underwater interaction measurements by using surface forces apparatus (SFA)

황동수

포항공과대학교 환경대학원

The surface forces apparatus (SFA) has been used for many years to measure the physical forces between surfaces, such as van der Waals, electrostatic forces, adhesion forces, ligand-receptor interactions, friction and lubrication force. Currently, the SFA technique is quite demanding for interdisciplinary area of physics, chemistry, biology, materials science, and chemical engineering. The SFA measures the magnitude and distance of the intermolecular forces between two atomically smooth surfaces by approaching, retracting or shearing from one another. Forces are measured with a resolution of 10nN and the separations are determined with 0.1 nm resolution by multiple beam interference fringes of equal chromatic order (FECO). A base surface for the SFA studies is usually mica but adsorbing or depositing a thin film of some other materials, i.e., lipid layers, metal oxides, polymer films including proteins and carbohydrate have been also used in the SFA. Here, an introduction to the SFA, the comparative analysis with AFM and its application to undwewater inteaction measurements will be discussed.

일시: 2014년 4월 16~18일(수~금) 3일간

장소: 일산KINTEX

발표코드: **KCS1-1**

발표분야: 국가와 기업이 원하는 과학기술 인재상

발표종류: 심포지엄, 발표일시: 목 10:00, 좌장: 석차옥

기술혁명시대와 연구자의 역할

김건

기초기술연구회

미정

일시: 2014년 4월 16~18일(수~금) 3일간
장소: 일산KINTEX
발표코드: **KCS1-2**
발표분야: 국가와 기업이 원하는 과학기술 인재상
발표종류: 심포지엄, 발표일시: 목 11:00, 좌장: 석차옥

SK가 원하는 과학 기술 인재상

곽병성

SK Innovation 기술원

미정

일시: 2014년 4월 16~18일(수~금) 3일간
장소: 일산KINTEX
발표코드: **KCS2-1**
발표분야: ICT 미래소재 심포지엄 (Flexible, Touch) - “감성은 부드럽게 Touch하고, 생각은 Flexible하게!”
발표종류: 심포지엄, 발표일시: 목 13:45, 좌장: 이승용

CdSe 기반 양자점(quantum dot, QD)의 합성과 응용 - 합성법 발전 과정과 해결할 문제점들

이진규

서울대학교 화학부

80 년대 초 CdS 에서 나노입자의 크기에 따른 에너지 준위의 변화가 관찰 된 이후, 이와 같은 반도체 나노입자들은 양자크기 효과 (quantum-size effect)의 대표적인 예로 연구되어 왔으며 이러한 나노미터 크기의 반도체 입자를 “양자점 (quantum dot, QD)”이라고 부른다.발광성이 큰 양자점의 합성법 개발과 함께 이들을 이용하여 다양한 소자로 응용하려는 연구가 활발히 진행되어 오고 있는데, 본 강연에서는 고효율의 발광성을 가지는 양자점 합성법이 개발되어 온 초기과정을 당시 AT&T Bell 연구소에서 함께 일을 했던 3 명의 선도적인 연구자들의 (Profs. Lois E. Brus, Paul A. Alivisatos, Moungi G. Bawendi) 업적을 살펴보면서 알아보도록 한다.또한, 그 동안 대량생산 등을 위한 어려움이 해결되어 온 과정을 살펴 보고, 이와 함께 현재까지 해결되지 못하고 있는 한계점 들에 대하여 논의하도록 한다.

일시: 2014년 4월 16~18일(수~금) 3일간

장소: 일산KINTEX

발표코드: **KCS2-2**

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

발표종류: 심포지엄, 발표일시: 목 14:20, 좌장: 이승용

공중합 캡핑제를 이용한 실버나노와이어 합성 및 응용

<u>서광석</u>

고려대학교 신소재공학부

터치스크린패널용 주요 소재인 투명전극 필름은 ITO 를 주로 사용하고 있으나, 유기 필름 위에 형성되어 있는 금속산화물의 강한 취성 때문에 보다 유연한 대체 재료 개발이 활발히 이루어지고 있다. 금속산화물을 이용한 전극재료를 대체할 수 있는 재료로는 CNT 와 그래핀 등의 탄소나노구조체, PEDOT 등의 전도성 고분자, 은 또는 구리 등의 금속 나노와이어 등이다.이들 중 최근 가장 활발하게 개발되고 있는 투명 전극용 재료가 은 나노와이어로서, 이는 전구체인 질산은 ($AgNO_3$)을 환원시켜 제조한다. 질산은을 환원용매를 이용하여 은 나노구조체를 형상함에 있어 캡핑제 (capping agent)라고 불리는 화합물을 사용하면 은이 한 방향으로 성장시켜 직경이 100 나노미터 미만인 은 나노와이어를 합성할 수 있다. 대표적인 캡핑제로는 폴리비닐피롤리돈 (polyvinylpyrrolidone), 이미다졸계 이온성 액체, polyethyleneoxide, sucrose 등이 있고, 환원 용매로는 에틸렌글리콜 (ethylene glycol) 등의 직접 환원시키는 용매 또는 물 등의 용매에 환원제를 혼합한 형태의 환원 용매계를 사용할 수도 있다. 또한 이들 캡핑제와 함께 사용하여 은 나노와이어의 직경을 더 가늘게 하고 길이를 더 길게 하는 방법도 이용되고 있다.본 발표에서는 공중합물을 이용한 새로운 캡핑제를 소개하고, 이용한 은 나노와이어 합성 및 이를 투명 전극 필름의 특성 등에 대하여 간략하게 소개하고자 한다.

일시: 2014년 4월 16~18일(수~금) 3일간
장소: 일산KINTEX
발표코드: **KCS2-3**
발표분야: ICT 미래소재 심포지엄 (Flexible, Touch) - “감성은 부드럽게 Touch하고, 생각은 Flexible하게!”
발표종류: 심포지엄, 발표일시: 목 15:10, 좌장: 양민수

AMOLED TV용 OLED 재료와 소자의 광특성 이해

권장혁

경희대학교 정보디스플레이학과

AMOLED 의 색특성은 일반 LCD 대비 그 순도가 매우 우수하여 방송규격 NTSC(National television System Committee)의 100% 색특성을 모두 표현해 주고 있다. 이는 사용되는 OLED 재료가 그 색특성이 매우 좋아서 그렇다고 생각할 수 있으나 실재로는 재료의 색순도는 NTSC 규격의 70% 수준밖에 되지 않는다. 현재 사용하는 OLED 소자의 색특성은 Micro-cavity 라는 광학현상을 이용하며 이를 이용하면 물질이 가지고 있는 특성을 최대한 활용하여 고색순도의 OLED 발광소자를 만들 수 있으며, 그 효율도 경우에 따라서는 매우 높일 수 있다. 본 심포지엄에서는 현재 AMOLED 에서 활용되는 Micro-cavity OLED 소자의 다양한 광특성을 이해하고 가장 최적으로 활용할 수 OLED 재료 및 기타 AMOLED 용 광학필름 재료에 대하여 토론하고자 한다.

일시: 2014년 4월 16~18일(수~금) 3일간

장소: 일산KINTEX

발표코드: **KCS2-4**

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

발표종류: 심포지엄, 발표일시: 목 15:45, 좌장: 양민수

유연 전자 소자 활용을 위한 박막 소재 및 소자 기술- 산화물 박막 트랜지스터에서부터 박막 봉지 재료까지

박진성

한양대학교 신소재공학과

올 1 월에 열린 2014 년 CES 에서는 중요한 핵심 기술들과 주제를 소개하였는데, 인터넷에 연결된 자동차, 입고 착용할 수 있는 ‘웨어러블 기술’, 대형 화면 등이 관심을 갖는 이슈가 되었다. 이 기술들 중에서 웨어러블 기술과 대형 화면은 향후 전자 소자 시장에서 빼 놓을 수 없는 제품의 핵심 역량으로 자리 잡을 것으로 판단된다. 현재 국내에서는 유연한 전자 소자에 적용하고 위한 제품들이 등장하고 있으며, 이들 중 선두주자는 디스플레이 분야이다. 특히, AMOLED 기반을 활용한 디스플레이 시장은 ‘플렉서블’이라는 화두를 맞춰가고 있으며, 이들에 대한 핵심 소재에서부터 다양한 공정 기술 그리고 제품이라는 하나의 축을 이뤄나가고 있다. 이번 발표에서는 최근 플라스틱 기반위에서 제작된 플렉서블 TFT 공정 기술들에 대하여 소개하고 향후 웨어러블 디스플레이로 가기 위한 핵심 기술들을 소개하고 한다. 디스플레이 분야에서 OLED 를 활용한 플렉서블 디스플레이는 주된 미래 핵심 기술로 판단하고 있으며, 이에 대응하고자 기존의 실리콘 반도체와 신규의 산화물 반도체 재료가 경쟁관계를 유지하고 있다. 또한, OLED 봉지 및 플렉서블 기판의 보호를 위하여 수분투습 방지용 박막 개발 연구가 크게 활성화 되고 있으며, 다양한 공정 기술을 활용하여 연구중이며, 이들 중에서 최근 연구를 진행하고 있는 원자층 증착 기반의 투습 방지 연구와 산화물 반도체 박막 트랜지스터의 유연 기반 적용 결과를 통해서 이슈와 가능성을 발표하고자 한다.

일시: 2014년 4월 16~18일(수~금) 3일간
장소: 일산KINTEX
발표코드: **KCS3-1**
발표분야: KCS Tutorial on Friday : Principle and Application of Graphene
발표종류: 심포지엄, 발표일시: 금 10:00, 좌장:

Electronic and optical properties of graphene: An introduction

박철환

서울대학교 물리천문학부

Many interesting properties of graphene arise from the linear electronic energy versus momentum relation. The origin of the linear electronic dispersion is the simple fact that graphene has two carbon atoms per unit cell. In this tutorial presentation, I will first explain the concept of pseudospin in graphene, which is up or down depending on which of the two carbon atoms the electron is localized at, and then discuss some of the basic electronic and optical properties of graphene.

일시: 2014년 4월 16~18일(수~금) 3일간

장소: 일산KINTEX

발표코드: **KCS3-2**

발표분야: KCS Tutorial on Friday : Principle and Application of Graphene

발표종류: 심포지엄, 발표일시: 금 10:40, 좌장:

Optical, electronic and scanning probe characterization of 2-dimensional crystals

류순민

경희대학교 응용화학과

Atom-thick 2-dimensional crystals such as graphene, h-BN and MoS_2 have not only led to many of new scientific findings but also hold substantial potential for applications in future molecular-scale integrated electronics, transparent conducting membranes, nanocomposites, etc. Further discovery of novel science and successful application require efficient synthesis/preparation and physical/chemical/mechanical manipulation of the low dimensional materials, which mandates reliable methods to characterize various materials properties such as morphological details, electronic and vibrational structures, chemical and mechanical properties, etc. In this tutorial, I will provide an overview of various optical, electronic and scanning probe-based analytical methods with a focus on optical spectroscopy of graphene.

일시: 2014년 4월 16~18일(수~금) 3일간
장소: 일산KINTEX
발표코드: **KCS3-3**
발표분야: KCS Tutorial on Friday : Principle and Application of Graphene
발표종류: 심포지엄, 발표일시: 금 11:40, 좌장:

Robust biosensors based on graphene oxide: towards practical implementation in biomedicine

민달희

서울대학교 화학과

To design practically useful biosensors based on new nanomaterials, one should understand and fully utilize chemical/physical properties to detect molecular changes during certain biochemical transformations in a biological system. Moreover, the new system should overcome limitations of conventional assay methods?detection limits, cost issues, labors, efficiencies, quantitativeness, reproducibility, etc. In this talk, I will introduce recent studies which harness graphene derivatives for developing bioanalytical platforms to quantitatively analyze various enzyme activities and biomarkers including helicase and microRNA. The systems rely on attractive interaction between graphene oxide and nucleic acids and fluorescence quenching by graphene oxide. Recently, we employed one of the graphene-based bioassay systems to anti-viral drug screening and identified potent hit compounds to treat hepatitis C. This study clearly shows that a new nanobio-technology can be routinely implemented in drug discovery, providing many advantages over conventional methods.

일시: 2014년 4월 16~18일(수~금) 3일간
장소: 일산KINTEX
발표코드: **KCS3-4**
발표분야: KCS Tutorial on Friday : Principle and Application of Graphene
발표종류: 심포지엄, 발표일시: 금 12:20, 좌장:

Synthesis and Applications of Large-Area Graphene

홍병희

서울대학교 화학부

The near explosion of attention given to graphene has attracted many to its research field. As new studies and findings about graphene synthesis, properties, electronic quality control, and possible applications simultaneous burgeon in the scientific community, it is quite hard to grasp the breadth of graphene history. At this stage, graphene’s many fascinating qualities have been amply reported and its potential for various electronic applications are increasing, pulling in ever more newcomers to the field of graphene. Thus it has become important as a community to have an equal understanding of how this material was discovered, why it is stirring up the scientific community and what sort of progress has been made and for what purposes. Since the first discovery, the hype has expediently led to near accomplishment of industrial-sized production of graphene. This tutorial covers the progress and development of synthesis and transfer techniques with an emphasis on the most recent technique of chemical vapor deposition, and explores the potential applications of graphene with industrial scale and quality that are made possible with various breakthroughs in synthesis and transfer techniques.

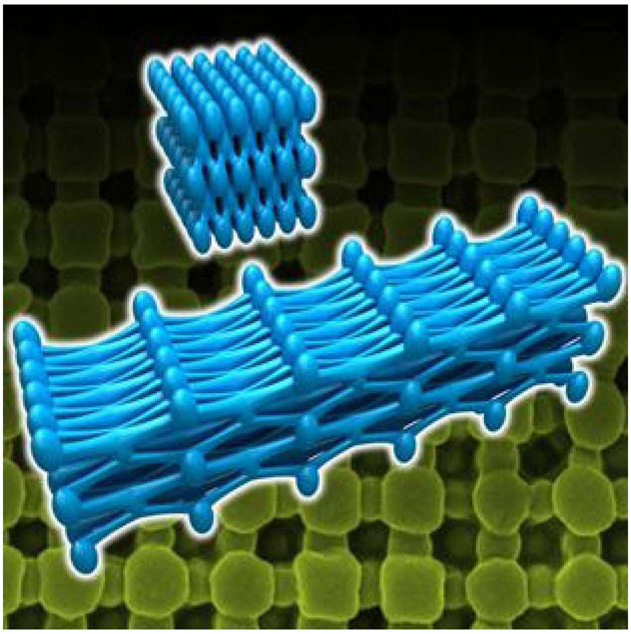
일시: 2014년 4월 16~18일(수~금) 3일간
장소: 일산KINTEX
발표코드: **KCS4-1**
발표분야: 한국다우케미칼 어워드 수상자 구두발표
발표종류: 심포지엄, 발표일시: 금 10:10, 좌장:

Extending the stretchability beyond intrinsic limit based on 3D nanostructures

박준용 전석우*

한국과학기술원(KAIST) 신소재공학과

Ever thought of electronics that can stretch like a rubber-band? Rarely is it possible to find electronic materials that can stretch, but if found, they could make sci-fi fantasies into reality. Skin tattoos that can replace your mobile devices, display screens that can be folded into your pocket, suits that can serve your computational needs all become possible through finding the right stretchable electronic material. But rather than creating such a material from scratch, it would be easier and more economical to convert an existing stretchable material into one that can stretch even more and also conduct electricity.Here we propose a new concept for realizing greatly enhanced stretchability beyond intrinsic limit of materials by structuring the materials in the form of 3D nanonetworks. The nanostructured material, poly(dimethylsiloxane) (PDMS), improves its stretchability up to 62% compared to bulk, solid PDMS. By infiltrating liquid metal into the 3D continuous network of periodic pores, the liquid metal and PDMS composite yields extremely high electrical conductivity (~24,100 S·cm^{-1}) even at the strains of >220%. Simple demonstration of LED arrays with the stretchable electrode proves the performance under extreme strains. Overall fabrication processes and stretching mechanism will be presented in this talk.



일시: 2014년 4월 16~18일(수~금) 3일간
장소: 일산KINTEX
발표코드: **KCS4-2**
발표분야: 한국다우케미칼 어워드 수상자 구두발표
발표종류: 심포지엄, 발표일시: 금 10:25, 좌장:

Deep-Blue Phosphorescence from Perfluoro Carbonyl-Substituted Iridium Complexes

이성훈 김슬옹[1] 신현 윤희준[1] 양기열[2] 권순기[1,*] 김윤희[3,*] 김장주[*]

서울대학교 재료공학부 [1]경상대학교 재료공학부 [2]경상대학교 화학교육과 [3]경상대학교 화학과

The new deep-blue iridium(III) complexes, $(TF)_2Ir(pic)$, $(TF)_2Ir(fptz)$, $(HF)_2Ir(pic)$ and $(HF)_2Ir(fptz)$, consisted of 2’,4’’-difluororphenyl-3-methylpyridine with trifluoromethyl carbonyl or heptafluoropropyl carbonyl at the 3’ position as the main ligand and a picolinate or a trifluoromethylated-triazole as the ancillary ligand, were synthesized and characterized for applications in organic light-emitting diodes (OLEDs). Density function theory (DFT) calculations showed that these iridium complexes had a wide band gap, owing to the introduction of the strong electron withdrawing perfluoro carbonyl group. Time dependent DFT (TD-DFT) calculations suggested that their lowest triplet excited state was dominated by a HOMO → LUMO transition and that the contribution of the metal-to-ligand charge transfer (MLCT) was higher than 34% for all four complexes, indicating that strong spin-orbit coupling exists in the complexes. The 10 wt% $(TF)_2Ir(pic)$ doped 9-(3-(9*H*-carbazole-9-yl)phenyl)-3-(dibromophenylphosphoryl)-9*H*-carbazole (mCPPO1) film exhibited the highest photoluminescence quantum yield 74 ± 3% among the films based on the four complexes. Phosphorescent OLEDs based on $(TF)_2Ir(pic)$ and $(TF)_2Ir(fptz)$ exhibited maximum external quantum efficiencies of 17.1% and 8.4% and Commission Internationale de l’Eclairage (CIE) coordinates of (0.141, 0.158) and (0.147, 0.116), respectively. These CIE coordinates represent some of the deepest blue emissions ever achieved from phosphorescent OLEDs with considerably high EQEs.

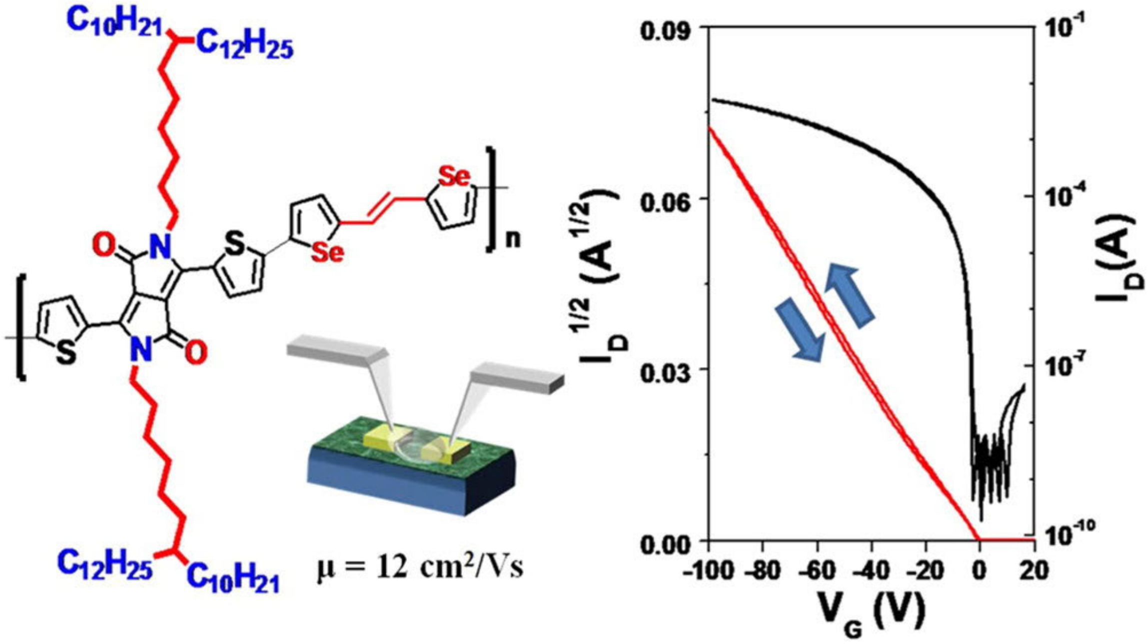
일시: 2014년 4월 16~18일(수~금) 3일간
장소: 일산KINTEX
발표코드: **KCS4-3**
발표분야: 한국다우케미칼 어워드 수상자 구두발표
발표종류: 심포지엄, 발표일시: 금 10:40, 좌장:

Record High Hole Mobility in Polymer Semiconductors via Side-Chain Engineering

강일 윤희준 정대성[1,*] 권순기[2,*] 김윤희[3,*]

경상대학교 고분자공학과 [1]중앙대학교 화학신소재공학부 [2]경상대학교 나노신소재공학부 [3]경상대학교 화학과

Charge carrier mobility is still the most challenging issue that should be overcome to realize everyday organic electronics in the near future. In this Communication, we show that introducing smart side-chain engineering to polymer semiconductors can facilitate intermolecular electronic communication. Two new polymers, P-29-DPPDBTE and P-29-DPPDTSE, which consist of a highly conductive diketopyrrolopyrrole backbone and an extended branching-position-adjusted side chain, showed unprecedented record high hole mobility of 12 $cm^2/(V \cdot s)$. From photophysical and structural studies, we found that moving the branching position of the side chain away from the backbone of these polymers resulted in increased intermolecular interactions with extremely short π-π stacking distances, without compromising solubility of the polymers. As a result, high hole mobility could be achieved even in devices fabricated using the polymers at room temperature.



C10H21
C12H25
Se
S
Se
O
N
N
O
S
n
C12H25
C10H21
μ = 12 cm²/Vs
0.09
0.06
0.03
0.00
I_D^1/2 (A^1/2)
10^-1
10^-4
10^-7
10^-10
I_D(A)
-100
-80
-60
-40
-20
0
20
V_G (V)

일시: 2014년 4월 16~18일(수~금) 3일간
장소: 일산KINTEX
발표코드: **KCS4-4**
발표분야: 한국다우케미칼 어워드 수상자 구두발표
발표종류: 심포지엄, 발표일시: 금 10:55, 좌장:

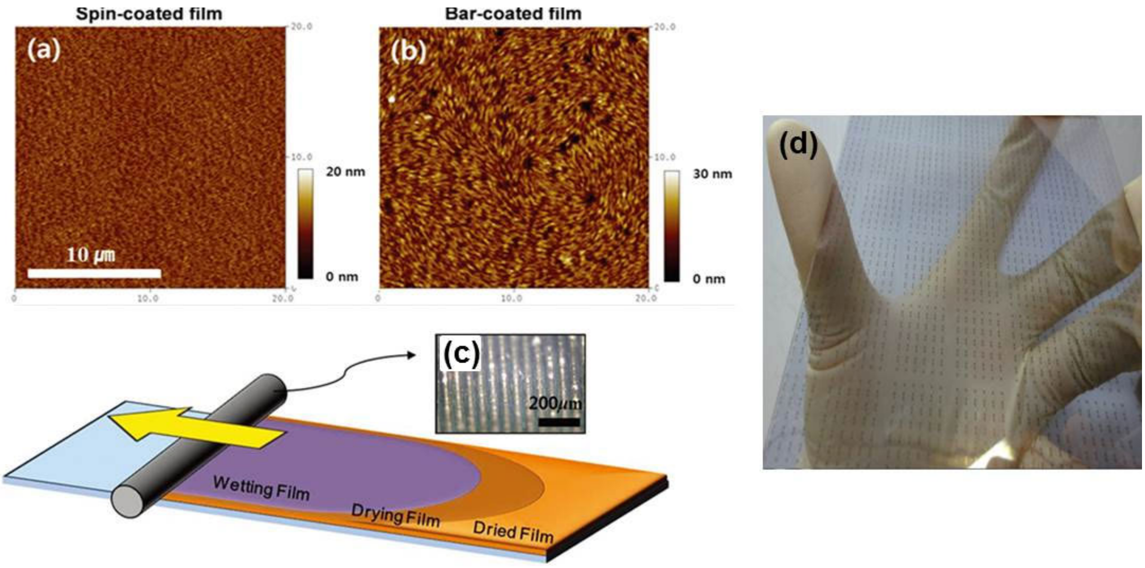
Simple Bar-Coating Process for Large-Area, High-Performance Organic Field-Effect Transistors and Ambipolar Complementary Integrated Circuits

김동윤 한현[1] 백강준[2] 김주환 곽선우[1] 김동유[*] 노용영[1,*]

광주과학기술원(GIST) 신소재공학과, 히거신소재연구센터 [1]동국대학교 융합에너지신소재공학과 [2]한국전기연구원 나노융합기술연구센터

We report a large-area, simple wire-bar?coating process as a suitable method for deposition of conjugated and insulating polymer films in OFET arrays and complementary ICs. The highly crystalline polymer semiconductor, PTVPhI-Eh, showed better crystalline morphology and the amorphous polymer semiconductor, (MEH-PPV) or PMMA, exhibited smoother film morphology when applied via the bar-coating process than by the spin-coating process. The best bar-coated OFETs with DPPT-TT showed a charge carrier mobility as high as 2.83 cm^2 V^{-1} s^{-1} and excellent device-to-device performance uniformity with standard deviation of 0.05~0.06 in 4 inch transistor arrays. Finally, we fabricated bar-coated ambipolar CMOS inverters (voltage gain ＞40) and ring oscillators (ROs) (oscillation frequency (fosc) of ~25 KHz) with a PTVPhI-Eh and CsF interlayer. We believe that this simple printing method is not only very effective for producing high performance device and circuits, but also highly compatible with roll-to-roll continuous manufacturing processes, which will enable fully printed large-area electronic and optoelectronic devices.

Figure. 1 (a) Top-surface AFM images of the PTVPhI-Eh semiconductor thin films deposited using (a) spin-coating and (b) bar-coating methods. (c) Schematic description of the bar-coating process. (d) Digital camera images of the bar-coated PTVPhI-Eh OFET array on a large size (10 cm × 10 cm)


Spin-coated film
Bar-coated film
(a)
(b)
20.0
10.0
0
20 nm
0 nm
30 nm
0 nm
10 μm
(c)
200μm
Wetting Film
Drying Film
Dried Film
(d)

일시: 2014년 4월 16~18일(수~금) 3일간
장소: 일산KINTEX
발표코드: **KCS4-5**
발표분야: 한국다우케미칼 어워드 수상자 구두발표
발표종류: 심포지엄, 발표일시: 금 11:10, 좌장:

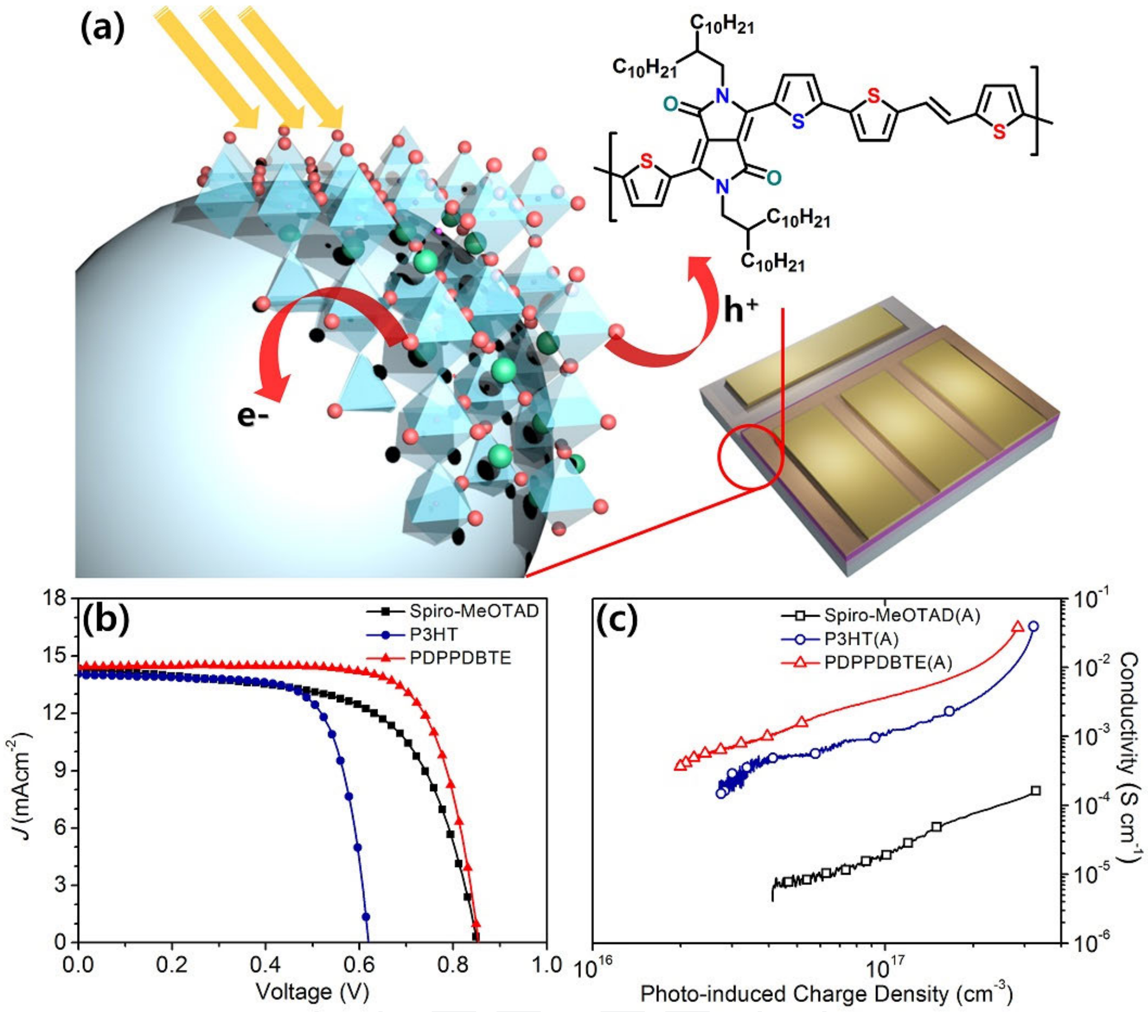
Diketopyrrolopyrrole-Containing Hole Transporting Conjugated Polymer for use in Efficient Stable Organic-Inorganic Hybrid Solar Cells based on a Perovskite

임종철 권영수 윤희준[1] 김윤희[1,*] 박태호[*]

포항공과대학교 화학공학과 [1]경상대학교 화학과

Poly[2,5-bis(2-decyldodecyl)pyrrolo[3,4-c]pyrrole-1,4(2H,5H)-dione-(E)-1,2-di(2,2’-bithiophen-5-yl) ethene] (PDPPDBTE) was successfully incorporated as a p-type hole transporting material in solid-state organic-inorganic hybrid solar cells. The excellent optical and electrical properties of organo-lead halide perovskite ($CH_3NH_3PbI_3$) nanocrystals used as a light harvester yielded a 9.2% power conversion efficiency (PCE) for the best-performing cell that exceeded the value (7.6%) obtained from the best hole conductor yet reported (2,2',7,7'-tetrakis(N,N-di-p-methoxyphenyl-amine)9,9'-spirobifluorene, spiro-MeOTAD). The high PCE was attributed to the optimal oxidation potential (5.4 eV) and excellent charge carrier mobility of the polymer. The hydrophobicity of the polymer prevented water permeation into the porous perovskite heterojunction, and long-term aging tests over 1000 hours confirmed the enhanced stability of the PDPPDBTE-based cells.

Figure 1. (a) D-π-A conjugated polymer successfully incorporated with perovskite-based organic-inorganic hybrid solar cells, outperforming the ever-best spiro-MeOTAD hole transporting material. (b) *J-V* curves of the hybrid solar cells made from spiro-MeOTAD, P3HT, and PDPPDBTE HTMs. (c) The effective conductivities of the HTMs ((A): including Li-TFSI and tBP additives).


(a)
$C_{10}H_{21}$
$C_{10}H_{21}$
N
O
S
S
S
S
N
O
$C_{10}H_{21}$
$C_{10}H_{21}$
h+
e-
(b)
Spiro-MeOTAD
P3HT
PDPPDBTE
J (mAcm-2)
Voltage (V)
0
3
6
9
12
15
18
0.0
0.2
0.4
0.6
0.8
1.0
(c)
Spiro-MeOTAD(A)
P3HT(A)
PDPPDBTE(A)
Conductivity (S cm-1)
Photo-induced Charge Density (cm-3)
10^16
10^17
10^-1
10^-2
10^-3
10^-4
10^-5
10^-6

일시: 2014년 4월 16~18일(수~금) 3일간

장소: 일산KINTEX

발표코드: **KCS4-6**

발표분야: 한국다우케미칼 어워드 수상자 구두발표

발표종류: 심포지엄, 발표일시: 금 11:25, 좌장:

Catalyst-free Direct Growth of Single to Few Layer Graphene on Germanium Nanowire for High Rate Lithium Battery Anode Material

김형기 최희철*

[1]IBS 원자제어 저차원 전자계 연구단, [2]포항공과대학교 화학과

Germanium (Ge) nanowire (NW) is one of the promising anode materials for high rate lithium (Li) ion battery due to its high specific capacity (1600 $mAhg^{-1}$) and fast Li ion diffusivity. Similar to silicon (Si) NW, however, Ge NW shows poor cyclability due to large volume expansion accompanied during lithiation-delithiation process. Herein we demonstrate that single to few layer high quality graphene grows directly on Ge NW (Gr@Ge NW) by chemical vapor deposition process without using conventional metal catalyst, and the Gr@Ge NW exhibits significantly enhanced cycle life (200 cycles) and specific capacity (1059 $mAhg^{-1}$) at high C-rate (4.0 C). The enhanced performance is attributed to tight encapsulation of Ge NW with high quality graphene that can suppress volume expansion and accomplish high electrical conductivity. More details will be discussed in the presentation.

일시: 2014년 4월 16~18일(수~금) 3일간
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Boosting the Ambipolar Performance of Diketopyrrolopyrrole-Selenophene Semiconducting Polymers via Hybrid Side-Chain Engineering

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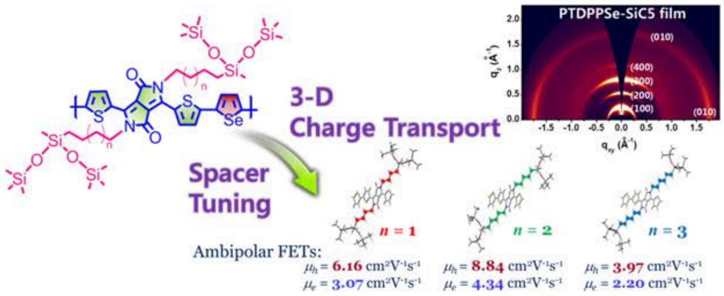
울산과학기술대학교(UNIST) 에너지공학과 [1]*포항가속기연구소* [2]*울산과학기술대학교(UNIST) 에너지공학과, 화학공학과*

Ambipolar polymer semiconductors are highly suited for use in flexible, printable, and large-area electronics as they allow for cost-effective fabrication of complementary circuits with high noise immunity and operational stability. Herein, we report solution-processable, high-performance, ambipolar polymer semiconductors that were developed via hybrid side-chain engineering of TDPP-selenophene copolymers with well-delocalized HOMO and LUMO isosurfaces over the conjugated backbone (PTDPPSe-SiCn, where n = 4-6). The siloxane-hybrid side chains allowed the formation of π-π stacking with face-on orientations and facilitated 3-D charge transport (Fig. 1). Furthermore, the molecular packing and charge transport were greatly affected by the length of the alkyl spacer in the hybrid side chain. The optimized 3-D charge transport of PTDPPSe-Si with pentyl spacers boosted ambipolar performance with significantly high hole and electron mobilities of 8.84 and 4.34 $cm^2\ V^{-1}\ s^{-1}$, respectively (Fig. 2). Our results provide guidelines for the molecular design of semiconducting polymers with hybrid side chains.



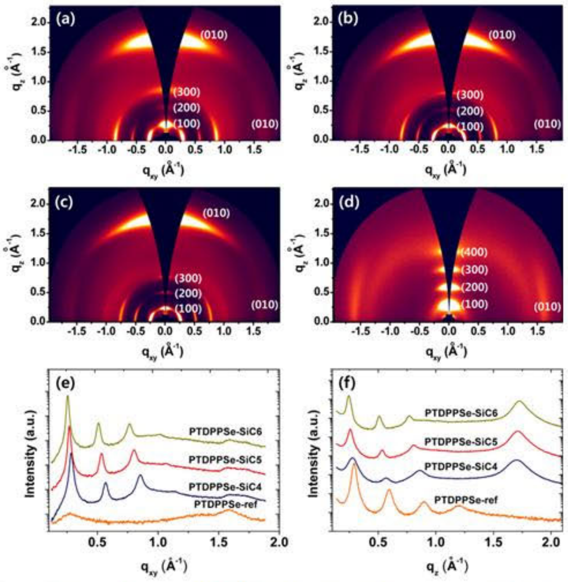


Fig. 1 GIXD images of drop-cast TDPPSe-based copolymer films annealed at 220 °C

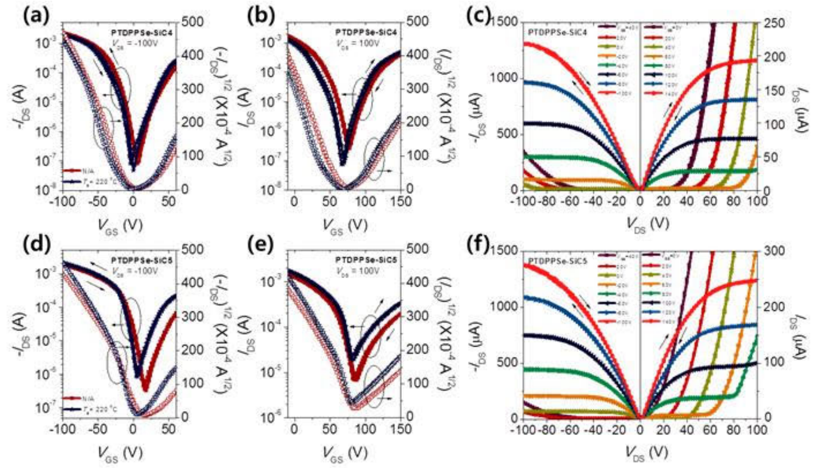


Fig. 2 The representative OFET performance of **PTDPPSe-SiC4** and **PTDPPSe-SiC5**.

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발표분야: 한국다우케미칼 어워드 수상자 구두발표

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Effects of octahedral to cuboctahedral shape transition in lead sulfide quantum dots Size-dependent air stability of lead sulfide quantum dots

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Lead sulfide nanocrystal quantum dots (NQDs) are a promising materials for application in solution-processed photovoltaic device due to their large bulk exciton Bohr radius, high carrier mobility, and dielectric constant. Here, we present a novel synthesis scheme to produce strongly confined PbS NQDs with a diameter 1.5 to 3 nm. We found that small sized PbS NQDs has better stability in air. We studied size-dependent surface chemistry between 1.5 and 7.5 nm in diameter using X-ray photoemission spectroscopy (XPS), inductively coupled plasma-atomic emission spectrometer (ICP-AES) measurements and density functional theory (DFT) calculations. Surprisingly, we discovered unexpected shape-transition from octahedral to cuboctahedral structure when size increases. This microscopic understanding of surface chemistry may be useful in the process of designing better stable PbS NQDs under ambient conditions in the future.

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Discovery of a Phosphor for Light Emitting Diode Applications and Its Structural Determination, Ba(Si,Al)$_5$(O,N)$_8$:Eu^{2+}

박운배 Satendra Pal Singh 손기선*

세종대학교 나노신소재공학과

Most of the novel phosphors that appear in the literature are either a variant of well-known materials or a hybrid material consisting of well-known materials. This situation has actually led to intellectual property (IP) complications in industry and several lawsuits have been the result. Therefore, the definition of a novel phosphor for use in light-emitting diodes should be clarified. A recent trend in phosphor-related IP applications, has been to focus on the novel crystallographic structure, so that a slight composition variance and/or the hybrid of a well-known material would not qualify from either a scientific or an industrial point of view. In our previous studies, we employed a systematic materials discovery strategy combining heuristics optimization and a high-throughput process to secure the discovery of genuinely novel and brilliant phosphors that would be immediately ready for use in light emitting diodes. Despite such an achievement, this strategy requires further refinement to prove its versatility under any circumstance. To accomplish such demands, we improved our discovery strategy by incorporating an elitism-involved non-dominated sorting genetic algorithm (NSGA-II) that would guarantee the discovery of truly novel phosphors in the present investigation. Using the improved discovery strategy, we discovered a Eu2+-doped AB5X8 (A = Sr or Ba, B = Si and Al, X = O and N) phosphor in an orthorhombic structure (A21am) with lattice parameters a=9.48461(3) Å, b=13.47194(6) Å, c=5.77323(2) Å, α=β=g=90°, which cannot be found in any of the existing inorganic compound databases.

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발표분야: New Horizons in Polymer Chemistry
발표종류: 구두발표, 발표일시: 금 10:00, 좌장: 박태호

Polymer Bulkheterojunction Solar Cells employing Triplet-Singlet Energy Transfer

권태혁

울산과학기술대학교(UNIST) 친환경에너지 공학부

Energy transfer has been widely exploited in organic light-emitting diodes to enhance emission efficiency and control the colour of emission, and in biosensor to increases signal-to-noise ratio. For efficient charge generation in organic solar cells, energy transfer has been emerged as a promising strategy because it can easily broaden a spectral response. Here, we present triplet-singlet energy transfer in polymer BHJ comprised of an iridium complex pendant with sodium cation as an energy donor, P3HT as an energy acceptor, and PCBM. With the iridium complex as an additive, we demonstrate a 20% increase of current density from 8.57 mA/cm2 to 10.40 mA/cm2, which corresponds to 3.3% of photo-conversion efficiency. One of main reason for the enhancement of current density comes from the efficient energy transfer from iridium complex to P3HT. The triplet-singlet energy transfer can be proved by enhancement of incident-photon-to-conversion efficiency (IPCE) spectrum between 350 to 410 nm, which is exactly overlapped with the absorption range of iridium complex. In addition, transient photoluminance studies reveal over 99% of triplet-singlet energy transfer efficiency. The other reason might be related with enhancement of morphology with iridium complex and/or increasing of diffusion length by triplet iridium complex. In summary, we suggest new types of energy donor additive for bulk heterojunction solar cells.

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Thermoresponsive Rod-Coil Diblock Copolymers Containing Poly(3-hexylthiophene)

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한국과학기술원(KAIST) 화학과

Poly(3-hexylthiophene) (P3HT) is one of the conducting polymers having good electrical properties. Self-assembly of P3HT has been studied intensively because the electrical properties of P3HT depend on the morphology formed by self-assembly of P3HT. P3HT usually shows self-assembled nano-fibril morphology whereas the nature of amphiphilic polymers lets them self-assemble into various nanostructure. This phenomenon has been studied recently, but it is not yet well understood. Poly(oligo(ethylene glycol) methyl ether methacrylate) (POEGMA) and poly(2-(2-methoxyethoxy)ethyl methacrylate) (PMEO2MA) are well known temperature responsive polymer showing lower critical solution temperature (LCST) in water. In addition, LCST point can be controlled by the ratio between OEGMA and MEO2MA. In this study, we synthesize amphiphilic diblock copolymers containing P3HT. Details on synthetic method and thermoresponsive properties of the amphiphilic diblock copolymers in solution will be presented.

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발표분야: New Horizons in Polymer Chemistry

발표종류: 구두발표, 발표일시: 금 10:25, 좌장: 박태호

Facile fabrication of NIR-responsive drug releasing system based on phase change material

이준석 김원종*

포항공과대학교 화학과

A phase change material (PCM) based NIR-sensitive drug releasing system was prepared. Blend of PCM and anticancer drug and gold nanorods covered with mesoporous silica (NR@MS) was nanoassembled to form a nanoparticle. Melting process of PCM driven by photothermal effect of AuNR caused fast release of loaded drug into the medium. Our system showed an effective cytotoxicity against various cell lines and intracellular release of drug was easily monitored by live cell imaging. Since our system does not require any complicated fabrication methods and PCM has a good capability to be blended with various hydrophobic drugs, it can be concluded that our system has a great potential for broad application in biomedical area as a delivery system for hydrophobic drugs with NIR-responsive behavior.

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발표분야: New Horizons in Polymer Chemistry
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Electrical memory characteristics of brush copolymer bearing carbazole and oxadiazole moieties in various compositions

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포항공과대학교 첨단재료과학부 [1]포항공과대학교 화학과 [2]National Taiwan University, Taiwan

Poly(N-vinylcarbazole) has gained attention because of its application in organic electronic devices as a hole transporting layer. Oxadiazole-containing polymers have also been extensively investigated as electron-transport materials. In this paper, brush copolymers bearing N-phenylcarbazole (PK) and 2-biphenyl-5-(4-ethoxyphenyl)-1,3,4-oxadiazole (BEOXD) moieties in various compositions were studied in detail, in particular their electrical memory characteristics, optical and electrical properties, morphological structures, and interfaces. Random copolymers with a high proportion of carbazole moieties exhibit static random access memory (SRAM) behavior, whereas random copolymers with a high proportion of oxadiazole moieties exhibit no electrical memory behavior at all. Moreover, the molecular orbitals and band gap can be tuned by changing the chemical composition. The novel memory characteristics of these copolymers originate primarily from the cooperative roles of the ambipolar PK and BEOXD moieties, which have different charge trapping and stabilization properties. The electrical memory behaviors were found to occur via a favorable hole injection from the electrode and to be governed by trap-limited space-charge limited conduction combined with ohmic conduction and local filament formation. Overall, the brush copolymers are very suitable active materials for the low-cost mass production of high performance, polarity-free digital memory devices that can be operated with very low power consumption, high ON/OFF current ratios, and high stability.

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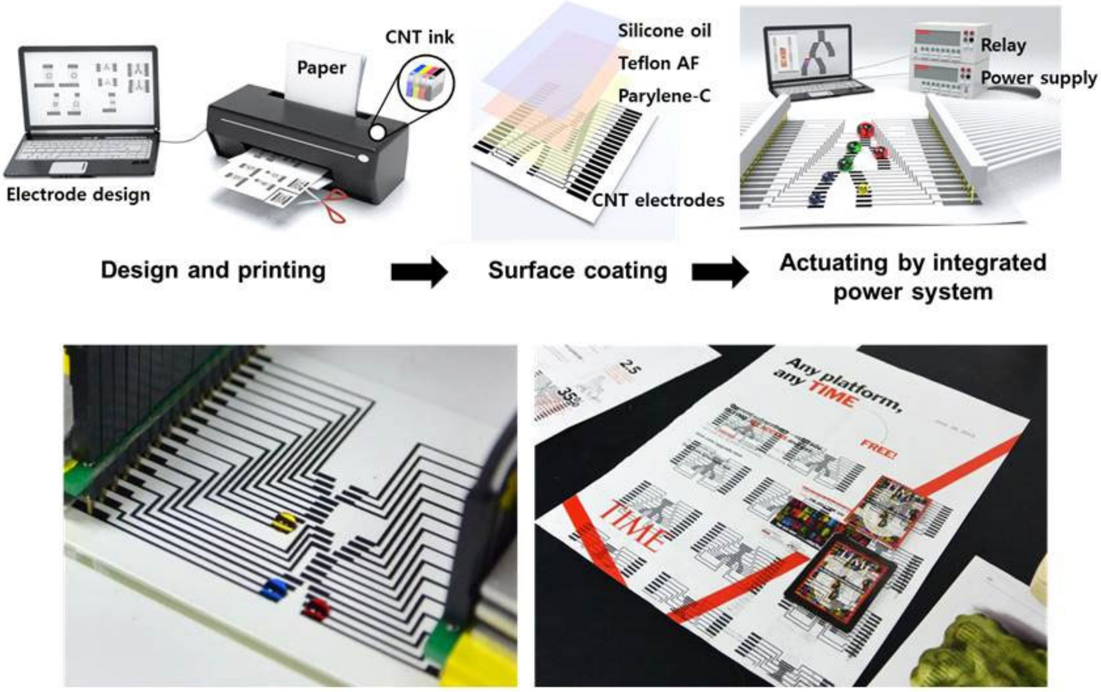
발표분야: New Horizons in Polymer Chemistry
발표종류: 구두발표, 발표일시: 금 10:45, 좌장: 박태호

Active Digital Microfluidic Paper Chips

고효진 이주미[1] 김용준 권오선* 신관우[2,*]

서강대학교 화학과 [1]서강대학교 화학 [2]서강대학교 화학과 및 바이오융합과정

Active digital microfluidic paper chips were fabricated which are low-cost, flexible, printable and easily disposable. Instead of using the passive capillary force on the pulp in the paper to actuate a continuous flow of a liquid sample, we used printed electrodes to transport a single, discrete drop or a group of digital liquid drops perfectly along programmed trajectories by electrowetting-on-dielectrics technique. We used inkjet printing with a commercial home/office inkjet printer and fabricated electrodes on commercially-available photo paper by using a homemade conductive carbon nanotube ink for this active paper open chip (APOC) system. The key advantage in fabricating APOCs is that electrode patterns can be designed and printed on paper quickly, finely and precisely without complicated wet-lab processes. We expect that this novel system will allow point-of-care production and diagnostic activities in the future.


CNT ink
Paper
Electrode design
Silicone oil
Teflon AF
Parylene-C
CNT electrodes
Relay
Power supply
Design and printing
Surface coating
Actuating by integrated power system
Any platform, any TIME
FREE!
TIME

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발표코드: **POLY.O-6**
발표분야: New Horizons in Polymer Chemistry
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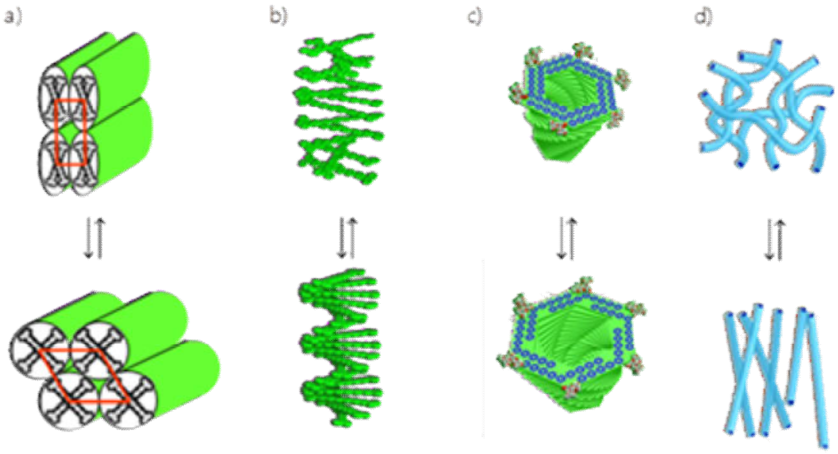
From Molecular Design to Magical Self-Assembled Nano-Materials

Zhegang Huang

Department of Chemistry, Harbin Institute of Technology, Harbin, China.

Supramolecular events take place through self-assembly process in which molecular modules spontaneously form ordered aggregates has been the subject of intense study as a means of creating intelligent materials and devices for nanotechnology. Among many self-assembling systems, aromatic rigid building blocks have proven to be particularly interesting due to their great potentials to construct smart soft materials. Because the self-assembly of the rod blocks arises mostly from subtle anisometric interactions, the small variations in local environments trigger rapid transformation of the equilibrium features. Along this line, we have constructed smart supramolecular systems by introducing oligoether dendrons into aromatic rod building blocks (Figure). Here, we will discuss from molecular design to synthesis and the exploration of smart nanostructures in aqueous and organic solution together with their practical implications.



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발표분야: New Horizons in Polymer Chemistry
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Elucidation for the silver-mediated fluorescence enhancement of DNA-templated AgNCs:a selective fluorogenic probe for the detection of nanomolar silver ions

이지현 김원종*

포항공과대학교 화학과

Silver ion mediated fluorescence enhancement on DNA-templated silver nanoclusters (DNA-AgNCs) is investigated as new, simple, sensitive and rapid type of silver ion detection probe. The DNA-AgNCs probe is prepared by chemical reduction method using air-saturated distilled water solution. Through analyzing the DNA-AgNCs probe using fluorescence spectroscopy and mass spectrometry, silver ion plays a role as a bridge for two DNA-AgNCs strands which emits strong green fluorescence as 43.9 % of quantum yield relative to Rhodamine 6G. Also utilizing the fluorescence enhancement of DNA-AgNCs by silver ions addition, we suggest a quantitative silver ion detection method which has low detection limit as 10 nM.

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발표분야: New Horizons in Polymer Chemistry
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Self-assembly of lipid-mimicking brush polymers in nanoscale thin films

김미희 이문호*

포항공과대학교 화학과

A series of well-defined poly(oxy(11-phosphorylcholineundecylthiomethyl)ethylene-ran-oxy(n-dodecylthiomethyl)ethylene) (PECH-PCm: m = 0?100 mol% phosphorylcholine (PC)) polymers were used to prepare nanoscale thin films that were characterized by synchrotron X-ray reflectivity (XR) analysis. The quantitative XR analysis provided structural insights into the PECH-PCm thin films. The PECH-PC0 polymer film formed a well-ordered in-plane oriented molecular multibilayer structure, whose individual layers consisted of two sublayers. One sublayer was composed of the fully extended backbones and inner part of the bristles, exhibiting a relatively low electron density, whereas the other sublayer was composed of a bilayer of the outer parts of the bristles without interdigitation. The PECH-PC100 polymer film also formed a well-ordered in-plane oriented molecular multibilayer structure, the individual layers of which were composed of four sublayers rather than two. The bristles in the layer were interdigitated in part via the zwitterionic interactions of the PC end groups. Surprisingly, regardless of the copolymer composition, the PECH-PCm random copolymer molecules in the thin films self-assembled to form a multilayered structure that resembled the structure formed by the PECH-PC100 polymer. These properties have not been observed in other conventional random brush copolymer films. The remarkable multibilayer structures originated from the zwitterionic PC end groups and their favorable interactions and interdigitated structures, which overcame any negative contributions caused by the heterogeneity of the bristles. The unique self-assembly properties of the PECH-PCm polymers always provide a PC-rich surface. The PECH-PCm random copolymers successfully mimicked the molecular bilayer structures formed by natural lipids.

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발표분야: New Horizons in Polymer Chemistry
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Well-Defined Dual Stimuli-Responsive Rod-Coil Block Copolymers

박창준 김상율*

한국과학기술원(KAIST) 화학과

Stimuli-responsive polymers have been of research interests due to their potential in many applications such as integrated optical devices, sensors and drug delivery agents. Especially, polymers which can respond to multiple stimuli have been of challenge because the polymers can show various self-assembly behavior by different stimuli. In this study, well-defined rod-coil block copolymers containing azobenzene moieties in rod block and 2-(2-methoxyethoxy) ethyl methacrylate (MEO_2MA) and oligo(ethylene glycol) methyl methacrylate (OEGMA) in coil block were synthesized. Through the chain-growth condensation polymerization and atom transfer radical polymerization, polymers with controlled molecular weights and polydispersity were produced. The rod-coil type block copolymers are expected to display light-responsive behavior by azobenzene moieties and temperature-responsive behavior by MEO_2MA and OEGMA moieties. Self-assembly behavior and stimuli-responsive behavior of polymers in aqueous solution will be presented.

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Self-assembly Behaviors of Diblock Copolypeptides in Nanoscale Thin Films

이진석 김경태 김미희 고용기 김영용[1] 김종현 이종찬 김용진[1] 이호열 이문호*

포항공과대학교 화학과 [1]포항공과대학교 첨단재료과학부

A series of diblock copolypeptides with various compositions (PBLG-b-PBCL) was synthesized through the living ring-opening polymerizations of g-benzyl-L-glutamate and 3-(benzyloxycarbonyl)-L-lysine N-carboxyanhydrides with the aid of a nickel catalyst system. Their chain conformations and morphologies in nanoscale thin films were characterized in detail by using infrared spectroscopy, atomic force microscopy, and in situ synchrotron grazing incidence X-ray scattering. In particular, quantitative X-ray scattering analysis was used to provide for the first time the morphological structures and orientation details of the diblock copolypeptides in thin films. Interestingly, the films are composed of two different rotationally isomeric hexagonally (HEX) packed cylinder structures that are preferentially oriented in the film plane. Further, the HEX structures consist of two substructural block units: one consisting of PBLG block chain cylinders and the other consisting of PBCL block chain cylinders. The block chains in the substructural units were found to interdigitate partially via the side groups. Thus the cylinders interdigitation takes place selectively between block chains of the same kind rather than between different kinds of block chains. It was also confirmed that this high interdigitation selectivity occurs in the blend films of the homopolypeptides. These results show that in diblock copolypeptide films such selective interdigitation can override any thermodynamic penalties associated with the high chain rigidity due to the a-helical conformation and the effects of confinement in the connected diblock architecture, which leads to phase separation and the formation of well-defined, integrated HEX cylinder structures.

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발표분야: New Horizons in Polymer Chemistry
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9,9'-Bifluorenylidene derivatives as non-fullerene type electron acceptor for organic photovoltaic cells

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부산대학교 [1]부산대학교 화학과

Fullerene derivatives are currently widely used as n-type semiconductors in solution-processed bulk-heterojunction (BHJ) solar cells because they have high electron affinity and good electron transporting ability. Fullerene and its derivatives, however, also have some drawbacks in real applications. The synthesis and purification of fullerene derivatives are difficult, and the manufacturing costs would be very high. To address these problems, non-fullerene electron acceptor materials from simple, minimal step, high yield, and inexpensive synthetic processes for application in organic photovoltaic cells (OPVs) are needed. In this study, we have investigated 9,9'-bifluorenylidene (9,9'BF) derivatives and 4,4'-bicyclopenta[def]phenanthrenylidene (4,4'BP) as non-fullerene electron acceptors for P3HT-based BHJ polymer solar cells. We have found that 9,9'BF derivatives can be used as non-fullerene electron acceptor for P3HT-based OPVs while similar devices using 4,4'BP do not show any photovoltaic effect. This can be related to the respective aromaticity and antiaromaticity of the reduced forms of 9,9'BF derivatives or 4,4'BP.

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발표코드: **POLY.O-12**

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Quentitative GIXS Analysis Complex Morphologies of Thin Films of an Asymmetric nine-arm Star Polymer

김종현 이문호*

포항공과대학교 화학과

An asymmetric nine-arm star polymer, (polystyrene) 3-(poly(4-methoxystyrene))3-(polyisoprene)3 (PS3-PMOS3-PI3) was synthesized, and and investigated the phase-separated structures and orientation details of its thin films by using in situ GIXS with a synchrotron radiation source. in situ GIXS measurements and quantitative data analysis were successfully carried out for the first time on thin films of the interesting asymmetric star polymer PS3-PMOS3-PI3. This analysis provided structural details of the thin films that are not easily obtained with conventional techniques. The CHCl3-annealed films were found to have a highly ordered, preferentially in-plane oriented. HEX structure consisting of truncated PS cylinders and truncated PMOS triangular prisms in the PI matrix. This complex three-phased HEX structure results from the phase separations of the asymmetric arms under the extreme conditions that their one-end was linked together and the confinement in the thin film by the air and substrate interfaces. The HEX structure is thermally stable up to near 190 °C. At 190 °C and higher temperatures (up to 220 °C), the HEX structure undergoes a partial rotational transformation that produces a 30°-rotated HEX structure. The thermally induced rotational structural isomer forms in a volume fraction of 23% and is preserved during the subsequent cooling run

일시: 2014년 4월 16~18일(수~금) 3일간
장소: 일산KINTEX
발표코드: **POLY.O-13**
발표분야: New Horizons in Polymer Chemistry
발표종류: 구두발표, 발표일시: 금 12:10, 좌장: 권태혁

Structure and properties of Self-assembled brush glycopolymers

이종찬 김미희 김경태 고용기 김영용[1] 김종현 이진석 김용진[1] 이문호[*]

포항공과대학교 화학과 [1]포항공과대학교 첨단재료과학부

A series of chemically well-defined brush glycopolymers having a polyoxyethylene backbone and bearing glycosyl and methyl end groups bristles was synthesized with various compositions. The glycopolymers were soluble in a variety of common solvents and were thermally stable up 200 oC. The brush polymer films formed multibilayer structures, displayed a glycosyl group-rich surface or a methyl group-rich surface or their mixture, depending on the bristle end group composition. The multibilayer structures were stabilized by the self-assembly of the bristles via lateral packing. The layers of which were stacked along the direction normal to the film plane. The glycosyl-rich surface enhanced the surface hydrophilicity and water sorption to a certain level; thus, the glycopolymer films easily formed a hydration layer to a certain depth on the film surface. The hydrophilic surfaces and hydration layer having good ability to prevent protein adsorption onto the brush glycopolymers and suppressed bacterial adherence while promoting mammalian cell adhesion in an in vivo mouse study. Also, glycopolymers displayed excellent biocompatibility.

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장소: 일산KINTEX
발표코드: **POLY.O-14**
발표분야: New Horizons in Polymer Chemistry
발표종류: 구두발표, 발표일시: 금 12:20, 좌장: 권태혁

Solution Processed Polymer/PCBM Bilayer Organic Photovoltaics Having Large Heterojunction Area

장윤희 김경곤*

이화여자대학교 화학나노과학과

Polymer solar cells utilize bulk heterojunction (BHJ) photoactive layer. The blended solution of electron donor and electron acceptor is used to form BHJ layer. However, forming nanoscale phase separations in the electron donor and acceptor is essential for facile charge carrier transport; this property is critical for the performance of BHJ solar cells. Consequently, the BHJ photoactive layer requires delicate control over the processing conditions (such as donor/acceptor blending ratio and processing additive) to obtain interpenetrated nanoscale phase separation between donor and accpetor. In contrast, bilayer heterojunction solar cell is more straightforward since each layer can be optimized independently by depositing polymer and C60 derivative layer sequentially. In this study, we report a new method to construct P3HT/PCBM bilayer having nanoscale HJ by utilizing co-solvent method. The photovoltaic performance of the bilayer film is studied with the device structure of PEDOT:PSS/P3HT/PCBM/LiF/Al. The roughened polymer layer forms nanoscale HJ with PCBM resulting in the enhanced charge separation and transport efficiency. The best P3HT bilayer devices show VOC of 0.62 V, JSC of 7.89 mA/cm2 and FF of 0.65, corresponding to PCE of 3.3%. Our bilayer solar cells show efficient charge separation and transport, and comparable efficiency to BHJ type solar cells.

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장소: 일산KINTEX
발표코드: **POLY.O-15**
발표분야: New Horizons in Polymer Chemistry
발표종류: 구두발표, 발표일시: 금 12:30, 좌장: 권태혁

Thickness and Composition Dependence of Electrical Memory Characteristics of Brush Polymers with Pendant Electron Donor and Acceptor Groups

김경태 이문호*

포항공과대학교 화학과

Electrical memory characteristics, optical and electrical properties, morphological structures, and interface characteristics of a series of brush copolymers bearing N-phenylcarbazole (PK) and 2-biphenyl-5-(4-ethoxyphenyl)-1,3,4-oxadiazole (BEOXD) moieties in various compositions were examined. Nanoscale thin films of the brush copolymers in devices were found to exhibit excellent unipolar electrical memory versatility, which can easily be tuned by tailoring the chemical composition and by changing the film thickness. Moreover, the molecular orbitals and band gap can be tuned by changing the chemical composition. The novel memory characteristics of these copolymers originate primarily from the cooperative roles of the PK and BEOXD moieties, which have different charge trapping and stabilization properties. The electrical memory behaviors were found to occur via a favorable hole injection from the electrode and to be governed by trap-limited space-charge-limited conduction, combined with ohmic conduction and local filament formation. Overall, the brush copolymers are very suitable active materials for the low-cost mass production of high performance digital memory devices that can be operated with very low power consumption, high ON/OFF current ratios, and high stability.

일시: 2014년 4월 16~18일(수~금) 3일간
장소: 일산KINTEX
발표코드: **POLY.O-16**
발표분야: New Horizons in Polymer Chemistry
발표종류: 구두발표, 발표일시: 금 12:40, 좌장: 권태혁

Synthesis and application of porous poly(amidoamine) particles via inverse suspension polymerization

이상화 김상율*

한국과학기술원(KAIST) 화학과

Poly(amidoamine)(PAMAM) can bind and separate heavy metal ions in aqueous solution. In this study, we developed a process to fabricate 50~300μm porous PAMAM particles by using silica particles. These porous particles were prepared via inverse suspension polymerization with N,N’-methylene bisacrylamide, ethylenediamine and silica particles. The silica particles were then removed by hydrofluoric acid to produce porous particles. SEM images showed many small pores in PAMAM particles. Detailed synthesis and characterization of the particles and their swelling ratio and metal ion absorption behavior will be presented.

일시: 2014년 4월 16~18일(수~금) 3일간
장소: 일산KINTEX
발표코드: **POLY.O-17**
발표분야: New Horizons in Polymer Chemistry
발표종류: 구두발표, 발표일시: 금 12:50, 좌장: 권태혁

Crystalline-Amorphous Diblock Copolymer Characteristics in Nanoscale Thin Films using Grazing incidence X-ray Scattering

김영용 이문호[1,*] 김상율[2,*] 김경태[1] 김미희[1] 고용기[1] 김종현[1] 이진석[1] 이종찬[1] 이호열[1]

포항공과대학교 첨단재료과학부 [1]포항공과대학교 화학과 [2]한국과학기술원(KAIST) 화학과

A diblock copolymer of crystalline polyethylene (PE) and amorphous poly(methyl methacrylate) (PMMA), PE69-b-PMMA92, was synthesized; this polymer is thermally stable up to 270 ?C. The structures of thermally annealed nanoscale thin films of the copolymer were measured in detail at various temperatures by using in-situ grazing incidence X-ray scattering (GIXS) with a synchrotron radiation source. Quantitative GIXS analysis showed that the PE and PMMA blocks undergo phase separation to produce a vertically oriented hexagonal PE cylinder structure in the PMMA matrix that is very stable up to 200 ?C, perhaps up to the degradation temperature. Furthermore, the PE block chains of the cylinder phase crystallize and undergo crystal growth along the cylinders' long axes; however, these lamellar crystals do not stack properly because of the limited space along the cylinders' short axes. As a result, the overall crystallinity is very low. The crystallization of the PE block chains in the diblock copolymer thin film is severely restricted in the diblock architecture by the confinement effects of the limited cylinder space and the anchoring of one end of the PE chain to the cylindrical wall interface.

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장소: 일산KINTEX
발표코드: **POLY.O-18**
발표분야: New Horizons in Polymer Chemistry
발표종류: 구두발표, 발표일시: 금 13:00, 좌장: 권태혁

High-performance N-channel Thin-Film Field Effect Transistors Based on Self-Assembly Polymer in Nanowire Suspension

고용기 이문호* 김용진[1]

포항공과대학교 화학과 [1]포항공과대학교 첨단재료과학부

A new electrontransport polymer, poly{[N,N ′-dioctylperylene-3,4,9,10-bis(dicarboximide)-1,7(6)-diyl]-alt -[(2,5-bis(2-ethyl-hexyl)-1,4-phenylene)bis(ethyn-2,1-diyl]} (PDIC8-EB), is synthesized. In chloroform, the polymer undergoes self-assembly, forming a nanowire suspension. The nanowire’s optical and electrochemical properties, morphological structure, and field-effect transistor (FET) characteristics are investigated [1]-[3]. Thin films fabricated from a PDIC8-EB nanowire suspension are composed of ordered nanowires and ordered and amorphous non-nanowire phases, whereas films prepared from a homogeneous PDIC8-EB solution consist of only the ordered and amorphous non-nanowire phases. X-ray scattering experiments suggest that in both nanowires and ordered phases, the PDIC8 units are laterally stacked in an edge-on manner with respect to the film plane, with full interdigitation of the octyl chains, and with the polymer backbones preferentially oriented within the film plane. The ordering and orientations are significantly enhanced through thermal annealing at 200 °C under inert conditions. The polymer film with high degree of structural ordering and strong orientation yields a high electron mobility (0.10±0.05 cm2 V?1 s?1), with a high on/off ratio (3.7 ×106), a low threshold voltage (8 V), and negligible hysteresis (0.5 V). This study demonstrates that the polymer in the nanowire suspension provides a suitable material for fabricating the active layers of high-performance n-channel FET devices via a solution coating process.

일시: 2014년 4월 16~18일(수~금) 3일간

장소: 일산KINTEX

발표코드: **INOR.O-1**

발표분야: Oral Presentation for Young Inorganic Chemists

발표종류: 구두발표, 발표일시: 금 10:00, 좌장: 이민형

Porous Proton Conducting Materials and Mechanistic Study

윤민영

가천대학교 글로벌캠퍼스 화학과

Proton conducting materials are an important component of fuel cells. Development of new types of proton conducting materials is one of the most important issues in fuel cell technology. The most studied and explored proton conducting materials are based on polymers, such as Nafion. Though the use of Nafion or Nafion-like polymer membranes is attractive, the high cost of the membranes still prevents a large scale use in many technologies. Newly developed porous proton conducting materials, including coordination polymers (CPs) or metal—organic frameworks (MOFs) have recently been investigated because of their designable and tunable nature. Herein, we present cucurbituril based organic molecular porous materials demonstrating the high and highly anisotropic proton conductivity. The isostructural organic porous materials showed different proton conductivity depending on the nature and amount of acid molecules present in the 1D channels. The highly anisotropic conduction behavior through the 1D channels of the porous CB[6] was studied by single crystal conductivity measurements. To the best of our knowledge, the porous CB[6] showed the highest anisotropic proton conductivity ($\sigma_{\parallel}/\sigma_{\perp} = 8600$) among the known proton conducting materials so far. For better understanding of proton conduction mechanism, proton conduction dynamics was investigated by ^{2}H NMR study and spectroscopical analysis. Details of our recent work will be presented.

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장소: 일산KINTEX
발표코드: **INOR.O-2**
발표분야: Oral Presentation for Young Inorganic Chemists
발표종류: 구두발표, 발표일시: 금 10:30, 좌장: 이민형

Photoinitiated multi-step charge separation and ultrafast charge transfer induced dissociation in a pyridyl-linked photosensitizer-cobaloxime assembly for aritificial photosynthesis

한원식

서울여자대학교

Using visible and near-infrared transient absorption spectroscopy to track distinct excited state, cation, and anion signals, a detailed kinetic analysis of photoinitiated multi-step charge separation and ultrafast charge transfer in donor?acceptor1?acceptor2 system is presented. The donor?acceptor1?acceptor2 ligand consists of a perylene (D) chromophore linked via a xylene bridge to a naphthalene-1,8-dicarboximide primary acceptor (NMI, A1) that is covalently linked to a 1,4,5,8-naphthalenetetracarboxylic diimide secondary acceptor (NDI, A2). Furthermore, coordination of pyridyl-substituted A1 ligand to the catalyst [Co(dmgBF2)2(L)2], where dmgBF2 = (difluoroboryl)dimethylglyoximato and L = water or a solvent molecule, yields a donor?bridge?acceptor?catalyst triad assembly. Detailed analysis of the electron transfer and dissociation dynamics of an integrated photosensitizer?catalyst system will inform the rational design of novel molecular assemblies that efficiently absorb photons, transfer electrons, and catalyze fuel-forming reactions.

일시: 2014년 4월 16~18일(수~금) 3일간

장소: 일산KINTEX

발표코드: **INOR.O-3**

발표분야: Oral Presentation for Young Inorganic Chemists

발표종류: 구두발표, 발표일시: 금 11:00, 좌장: 이민형

Conformational Design with π-Conjugated Molecules: Evolving Strategies for Metal Binding and Detection

이동환

서울대학교 화학부

전자가 비편재화된 유기분자 구조의 고유한 전기적/광학적 성질을 이용한 기능성 분자나 조합체에 관한 연구가 활발히 이루어지고 있다. 아릴렌-에티닐렌의 기본 구조 모티프에 기반한 파이-컨쥬게이션의 경우, 탄소-탄소 결합의 뒤틀림으로 인한 분자구조의 변화를 이용하여, 금속 이온의 결합을 포함한 다양한 화학적 신호를 쉽게 감지할 수 있는 전기적/광학적 성질의 변화로 잘 연계시킬 수 있다. 헤테로원자에 기반한 적절한 작용기나 리간드를 파이-컨쥬게이션 분자 골격에 도입함으로써, (i) 금속 이온과의 가역적 결합을 통한 형광성의 변화, (ii) 금속 이온에 의한 비가역적 화학반응에 의한 형광성의 증가, (iii) 금속 이온을 템플리트로 만들어진 용액상의 응집체에 대한 구조/분광학적 정보 수집 등에 이용할 수 있다. 이와 같이 다양한 분야에 응용할 수 있는 기능성 파이-컨쥬게이션 분자의 설계와 구조-물성-반응성 사이의 긴밀한 상관관계를 중심으로, 지난 몇 년간 본 연구실에서 수행해 왔던 연구주제들을 소개하고자 한다.

일시: 2014년 4월 16~18일(수~금) 3일간

장소: 일산KINTEX

발표코드: **INOR.O-4**

발표분야: Oral Presentation for Young Inorganic Chemists

발표종류: 구두발표, 발표일시: 금 11:40, 좌장: 윤민영

Novel Dielectric Materials for High Performance and Low-Voltage Thin-Film Transistors: Organic-Inorganic Hybrid Blends and Multilayers

하영근

경기대학교 화학과

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

일시: 2014년 4월 16~18일(수~금) 3일간

장소: 일산KINTEX

발표코드: **INOR.O-5**

발표분야: Oral Presentation for Young Inorganic Chemists

발표종류: 구두발표, 발표일시: 금 12:10, 좌장: 윤민영

Dual Sensing of Zn(II) Cation and Fluoride Anion Using Terpyridine-Triarylborane Conjugates

이영훈 이민형[1,*]

울산대학교 기초과학연구소 [1]울산대학교 화학과

Molecular receptors capable of effectively recognizing charged species have been actively studied in the field of supramolecular chemistry. Among them, heteroditopic receptors that contain two disparate recognition sites for both cations and anions may be good candidates for sensing purposes because they can exhibit enhanced affinity for target species in comparison to the corresponding monotopic receptors probably due to allosteric effects and favorable electrostatic interactions between the cobound ions in ion-pair receptors. In this regard, we have designed and synthesized a series of novel ditopic terpyridine-triarylborane conjugates where 4′-ethynylterpyridine is linked to the para-, meta-, and ortho-positions of the phenyl ring of dimesitylphenylborane. Their dual binding behavior toward Zn(II) cation and fluoride anion have been investigated in detail by single crystal X-ray structural determination, spectroscopic analysis, and theoretical calculation. All complexes show the formation of a 1:1 adduct between ZnCl2 and each conjugate with a distorted trigonal bipyramidal geometry. The addition of Zn(II) ion led to the red shifts of absorption and emission bands due to intramolecular charge transfer transition while both bands are quenched upon addition of fluoride anion.

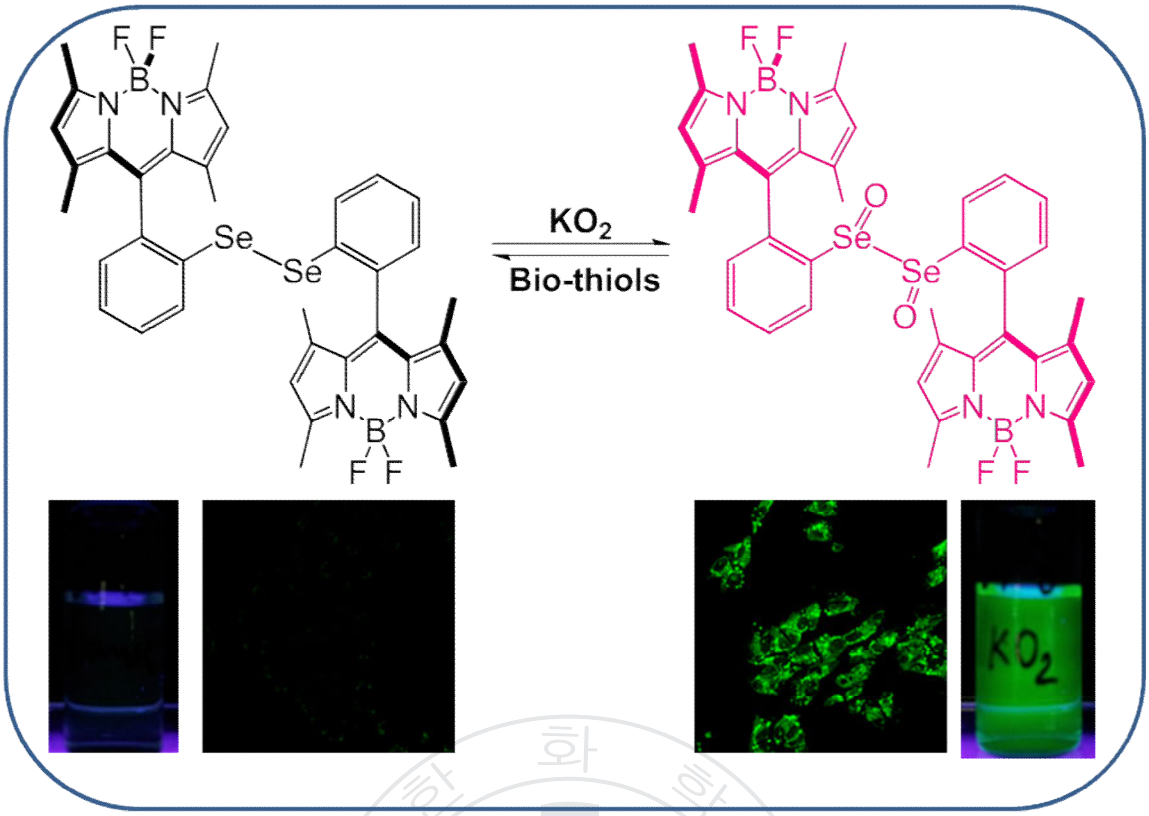
일시: 2014년 4월 16~18일(수~금) 3일간
장소: 일산KINTEX
발표코드: **INOR.O-6**
발표분야: Oral Presentation for Young Inorganic Chemists
발표종류: 구두발표, 발표일시: 금 12:35, 좌장: 윤민영

Selective, Sensitive and Reversible Detection of ROS with a Novel Chalcogen-based Molecular Probes

MANJARESUDESHTULSHIRAM D.G.Churchill[1,*]

기초과학연구원(IBS) 분자활성 촉매반응 연구단 [1]한국과학기술원(KAIST) 화학과

Reactive oxygen species (ROS) exist in, and are utilized by biology and neurobiology, yet they constitute so-called oxidative stress when present in unwanted excess. This may be a major contributing factor for diseases such as diabetes, cancer and molecular neurodegenerative disorders such as Alzheimer’s and Parkinson’s disease. Reactive oxygen species (ROS) are often mentioned in conjunction with nitrogen-based analogues (RNS), and include various species such as HOCl, OH˙, H2O2, NO, ONOO-, O2˙-, tBuOOH and, tBuO˙. Sensitive and selective detection of such species with fluorescence microscopy requires discrete synthetic molecular design and syntheses that are straight-forward and good yielding. A great number of novel heterocycles bearing single or multiple nitrogen, oxygen, sulphur, selenium or tellurium sites have been investigated over the years; many of these are heterocyclic pharmacophores bearing biological activity. One important challenge for organochalcogen chemists has been to synthesize novel heterocyclic systems and dichalcogen-based reversible probes. Thus, in this work, we are presenting novel annulated BODIPY chalcogenide (Se, Te) systems and diselenide-based BODIPY probes synthesized from their respective bis(o-formyl-phenyl)dichalcogenide intermediates. The annulated BODIPY selenide product was confirmed by X-ray diffraction. The red-shifted annulated BODIPY telluride version was found to be sensitive and selective for hypochlorite, reversible upon treatment with bio-thiols in water. Methyl-substituted BODIPY-based diselenide probe was found to be sensitive and selective for superoxide in giving [-Se(O)Se(O)-] oxidation. Probing was reversible through bio-thiols. Practical medicinal utility of BODIPY-based diselenide was demonstrated in MCF-7/ADR cancer cells for the detection of superoxide.


F F
B
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일시: 2014년 4월 16~18일(수~금) 3일간

장소: 일산KINTEX

발표코드: **PHYS.O-1**

발표분야: General Oral Presentation

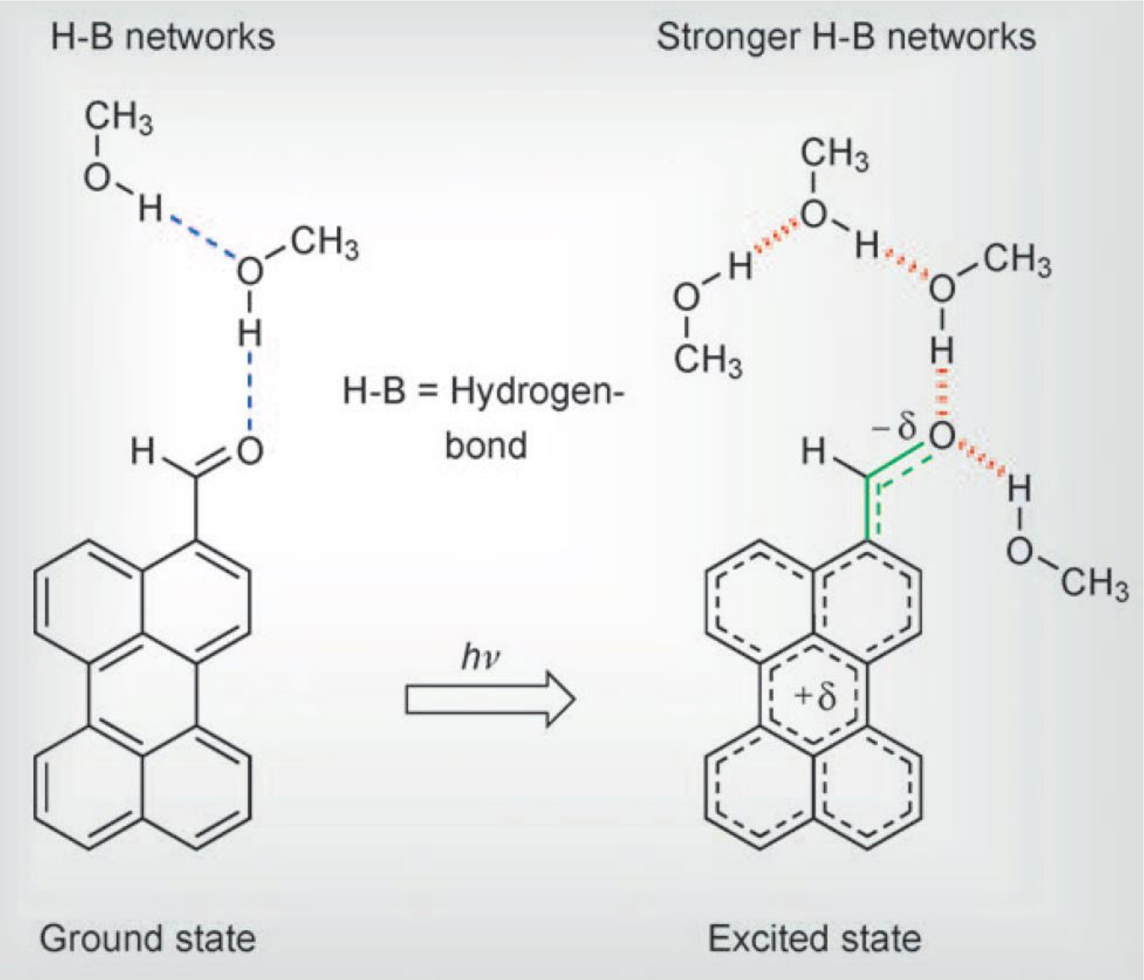
발표종류: 구두발표, 발표일시: 금 10:00, 좌장: 이남기

The role of alcohol clusters in elementary excited-state chemical reactions revealed by femto-to-picosecond-resolved electronic spectroscopy

권오훈

울산과학기술대학교 자연과학부 화학과

The nature of amphiprotic liquid to form hydrogen (H)-bond networks is essential for efficient proton solvation and migration. For example, the proton affinity of water, a fundamental medium to many chemical and biological processes, greatly increases by the formation of tetrahedrally coordinated H-bond network to solvate a proton in the form of an Eigen-type cation ($H_3O^+\cdot 3H_2O$), a solvated hydronium ion (1). According to Grotthus mechanism, the hydronium core can rapidly diffuse over a long distance without the need for any specific cation to travel more than an order of a single bond. Another liquid of strong interest is methanol. Methanol is the simplest stable organic molecule with H-bonding capability. Compared to water the presence of the methyl group leaves a methanol molecule two H-bonding sites, one of which for H-bond donation and the other for H-bond acceptance. This leads to the formation of H-bond networks in (quasi) one-dimensional linear fashion. Recently, the importance of alcohol not only as a nonspecific, passive dielectric medium, but also as an active participant in reactions has been pointed out. Here, we present the key role of clustered alcohol molecules in a series of elementary chemical reactions, as a catalyst (2), a Brønsted base (3), and an electron acceptor (4), utilizing femto-to-picosecond fluorescence spectroscopy. References1.Kwon, O.-H.; Mohammed, O. F. Phys. Chem. Chem. Phys. 2012, 14, 8974.2.Kwon, O.-H.; Lee, Y.-S.; Yoo, B. K.; Jang, D.-J. Angew. Chem. Int. Ed. 2006, 45, 415.3.Kim, T.-G.; Ajitha, M.-J.; Jung, Y.; Kwon, O.-H., submitted.4.Mohammed, O. F.; Kwon, O.-H.; Othon, C. M.; Zewail, A. H. Angew. Chem., Int. Ed. 2009, 48, 6251.


H-B networks
Stronger H-B networks
CH_3
O
H
O
CH_3
H
H
O
H-B = Hydrogen-bond
$h\nu$
−δ
+δ
Ground state
Excited state

일시: 2014년 4월 16~18일(수~금) 3일간
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발표코드: **PHYS.O-2**
발표분야: General Oral Presentation
발표종류: 구두발표, 발표일시: 금 10:15, 좌장: 이남기

Emerging beam resonances in atom diffraction from a reflection grating

조범석

울산과학기술대학교(UNIST) 나노생명화학공학부

We report on the observation of emerging beam resonances, well known as Rayleigh-Wood anomalies and threshold resonances in photon and electron diffraction, respectively, in an atom-optical diffraction experiment. Diffraction of He atom beams reflected from a blazed ruled grating at grazing incidence has been investigated. The total reflectivity of the grating as well as the intensities of the diffracted beams reveal anomalies at the Rayleigh angles of incidence, i.e., when another diffracted beam emerges parallel to the grating surface. The observed anomalies are discussed in terms of the classical wave-optical model of Rayleigh and Fano

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발표종류: 구두발표, 발표일시: 금 10:30, 좌장: 이남기

SERS Hot Spot Formation with Thiol Functionalized Cucurbit[n]uril

김남훈 윤경원[1] 김지홍[1] 김기문[1,*]

기초과학연구원 복잡계자기조립연구단 [1]포항공과대학교 화학과

We developed a new strategy for the generation of surface-enhanced Raman scattering (SERS) hot spots by anchoring a suitable target molecule in a close proximity to the metal surface/nanoparticle using the host-guest chemistry of cucurbit[6]uril (CB[6]). Ag nanoparticles residing above a bulk Ag substrate was prepared, which is almost as an effective SERS substrate as two closed coupled silver nanoparticles. The role of thiol-CB[6] is a linker which connects Ag nanoparticle and a bulk Ag substrate with a reproducible gap distance forming strong Ag-S bonds. The gap distance between Ag nanoparticle and Ag substrate is close enough for a strong SERS signal. The structure of these nanostructures was investigated by transmission electron microscopy (TEM), atomic force microscopy (AFM), IR, UV-Vis spectroscopy, and X-ray photoelectron spectroscopy (XPS). IR and XPS measurements confirm the vertical geometry of thiol CB[6] on metal surface indicating that the CB[6] pore is open. These open CB[6] pore can interact with several guest molecules very selectively generating very strong SERS signal of guest molecules. Spermine-functionalized dye molecules were used as a guest molecule and a Raman report molecule. This system provides reproducible SERS hot spot having chemical selectivity via the host-guest interaction of CB[6] and spermine. Using the polarization dependant SERS mapping technique, we observed the single molecule behavior of the spermine-functionalized dye molecules.

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발표코드: **PHYS.O-4**

발표분야: General Oral Presentation

발표종류: 구두발표, 발표일시: 금 10:45, 좌장: 이남기

STORM for live cells: super-resolution fluorescence microscopy via single-molecule localization

심상희

울산과학기술대학교(UNIST) 생명공학과, 화학과

“Super-resolution” fluorescence microscopy has overcome the diffraction limit of optical microscopes over an order of magnitude. One major group of such methods utilizes photoswitching probes for separating fluorophores in time, thereby localizing single molecules at high precision. This group was first introduced by the names of STORM (stochastic optical reconstruction microscopy) and PALM (photoactivated localization microscopy). STORM/PALM has demonstrated up to 10-nm resolution as well as multicolor and 3D capabilities using standard optical microscopes.

Here, I will present STORM imaging methods for living cells. Proteins in live cells were imaged with photoswitchable cyanine dyes whose brightness and fast switching enabled 3D resolutions of 30-50 nm within 1-2 seconds. Membranes in live cells were stained with small-molecule probes that allowed us to resolve previously obscured details on dynamics of the plasma membrane, the endoplasmic recticulum (ER) and mitochondria. The live-cell STORM methods open new windows for visualizing nanometer-scale dynamics *in vivo*.

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발표분야: General Oral Presentation
발표종류: 구두발표, 발표일시: 금 11:00, 좌장: 이남기

Time-Dependent Density Functional Theory Studies of Optical Properties of Au Nanoparticles: Octahedra, Truncated Octahedra, and Icosahedra

배균택

충북대학교 사범대학 화학교육과

The optical absorption properties of gold nanoparticles are investigated theoretically in the study of plasmonic optical properties. A Time-Dependent density functional theory (TDDFT) approach is employed to determine optimized structures and excitation energy calculations for a set of three structural shapes: octahedra, truncated octahedra, and icosahedra (Aun, n=6-85) in various charge states that correspond to shell closing. Octahedral Aun clusters with n=6, 19, 44, 85, truncated octahedral Aun clusters with n=13, 38, 55, 79, and icosahedral Aun clusters with n=13, 43, 55 are calculated. The optimization calculations are used with the BP86/DZ.4f level of theory and the excitation energy calculations are used with the LB94 functional. All calculations are performed using the ADF code.

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발표코드: **PHYS.O-6**
발표분야: General Oral Presentation
발표종류: 구두발표, 발표일시: 금 11:20, 좌장: 권오훈

Investigations of transcriptional dynamics of T7 RNA polymerase in live E. coli cells

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포항공과대학교 물리학과 [1]포항공과대학교 I-BIO(시스템생명공학부) [2]포항공과대학교 시스템생명공학부/물리학

Transcription, a reaction of synthesizing mRNA, is the key process for gene expression regulation in living cells. Most studies on transcription have been done outside cells using purified RNA polymerases (RNAP). Thus, the dynamics of RNAP in living cells, especially in the presence of vast chromosomal DNA and other cellular proteins, such as ribosome, are still poorly understood. Here we applied single fluorescent protein imaging to probe the dynamics of RNAP in E. coli, using T7 RNAP as a model system. We measured the elongation rate of T7 RNAP in living cell and found that it takes nearly 60 min for one T7 RNAP to generate one mRNA. Transcription by T7 RNAP is also coupled with translation that the absence of ribosomal binding site (RBS) on RNA reduces the transcription rate by half. However, there was no change in the elongation rate of T7 RNAP by the coupling with translation. Importantly the location of the transcribing gene is moved to membrane side, which is controlled by the translation. Thus our result demonstrates a new model on the bacterial transcription that translation by ribosome induces the dynamic movement of the transcribing gene to membrane side, which increases the transcription rate.

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발표분야: General Oral Presentation
발표종류: 구두발표, 발표일시: 금 11:30, 좌장: 권오훈

Structure-Property Relationship of Perylene Bisimide Macrocycles Probed by Atomic Force Microscopy and Single-Molecule Fluorescence Spectroscopy

이지은 김동호*

연세대학교 화학과

Properties of a series of acetylene-linked perylene bisimide (PBI) macrocycles with different ring size composed of three to six PBI dyes were investigated by atomic force microscopy (AFM) and single-molecule fluorescence spectroscopy in a condensed phase. It was demonstrated that the structures of PBI cyclic arrays (CNs, N = 3, 4, 5, and 6) become distorted with increasing the ring size through molecular dynamics (MD) simulations (PM6-DH2 method) and AFM height images of CNs on highly ordered pyrolytic graphite (HOPG) surface. The MD simulations showed that only C5 and C6 rings are highly flexible molecules whose planarization goes along with a significant energetic penalty. Accordingly, both molecules did not show ordered adlayers on a HOPG surface. In contrast, C3 and C4 are far more rigid molecules leading to well-ordered hexagonal (C3) and rectangular (C4) 2D lattices. At the single-molecule level, we showed that the fluorescence properties of single CNs are affected by the structural changes. The fluorescence lifetimes of CNs became shorter and their distributions became broader due to the structural distortions with increasing the ring size. Furthermore, the CNs of smaller ring size exhibit a higher photostability and an efficient excitation energy transfer (EET) due to the more well-defined and planar structures compared to the larger CNs. Consequently, these observations provideevidence that not only PBI macrocycles are promising candidates for artificial light-harvesting systems, but also the photophysical properties of CNs are strongly related to the structural rigidity of CNs.

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발표코드: **PHYS.O-8**
발표분야: General Oral Presentation
발표종류: 구두발표, 발표일시: 금 11:40, 좌장: 권오훈

Understanding the Role of Denaturation and Hydrophobic Interaction in Amyloid Fibrillation of Insulin

최태수 김준곤*

포항공과대학교 화학과

Amyloid fibrillation is an abnormal aggregation phenomenon of amyloidogenic proteins, which are highly correlated with senile disorders such as Alzheimer’s disease, Parkinson’s disease, type 2 diabetes, and spongiform encephalopathy. The fibrillation process of amyloidogenic proteins is initiated by exposing hydrophobic residues to solvent molecules (denaturation of protein), and amyloid self-assembly occurs between hydrophobic residues of proteins (hydrophobic interaction). In the present study, we investigate the role of protein-solvent interaction to understand a correlation between denaturation and hydrophobic interaction during the fibrillation process of insulin. Thioflavin T assay and transmission electron microscopy (TEM) images exhibit that binary mixtures of water and formamide derivatives promotes the formation of insulin fibril compared with water. However, non-aqueous solutions of formamide derivatives suppress the formation of insulin fibril with much longer lag time than the presence of water. Solution small-angle X-ray scattering (SAXS) combined with molecular dynamics (MD) simulation suggests that fibrillation kinetics of insulin in the binary mixtures is highly promoted by the denaturation of B11-B17 core sequence residues. Differential scanning calorimetry (DSC) shows that the presence of water is crucial for intermolecular protein-protein hydrophobic interaction. These results indicate that both denaturation and hydrophobic interaction plays an important role in the amyloid fibrillation.

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발표분야: General Oral Presentation
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Controlling Surface Structure and the Au(111) Work Function by Halo-Substituted Aromatic Thiol Self-Assembled Monolayers

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한양대학교 화학과 [1]RIKEN [2]RIKEN, TITech

Self-assembled monolayers (SAMs) with strong electron-withdrawing groups such as halo-substituted aromatic SAMs are found to decrease the barrier for electron or hole injection into the organic semiconductor. For this application, it is important to understand SAM structure of halo-substituted aromatic thiols on metal surface. We observed the surface structure, thermal desorption properties, and electronic properties of halo-substituted aromatic thiol SAMs on Au(111). From the scanning tunneling microscopy (STM) observation, we found that high immersion temperature is powerful method to fabricate the highly well-ordered SAMs. And from the observation of work function changes of metal surface modified with SAMs, it was revealed that the dipole moment normal component to the surface is crucial factor in determining the work function changes of metal surface modified with SAMs. In the case of tetrafluorobenzenethiol (TFBT) SAMs formed at 50 °C, the surface structure was dramatically changed and the quality of molecular ordering was greatly improved compared to that formed at room temperature. High-resolution STM images clearly revealed for the first time that TFBT SAMs formed at 50 °C were composed of highly, 2D ordered domains, which can be described as a $(2\sqrt{3} \times 8\sqrt{2})R45^\circ$ structure. Varying ratio of vertical and parallel component of SAM dipole moment by 2D structural control of SAMs opens up the new possibility for modification of the electrode work function deposited with SAMs.

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발표분야: General Oral Presentation
발표종류: 구두발표, 발표일시: 금 12:00, 좌장: 권오훈

Systematic preparation of colloidal Ag nanoparticles and application to SERS of biphenyl derivatives

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강원대학교 화학과

Optimized parameters to produce aggregated silver colloidal nanoparticles in solution for the effective surface-enhanced Raman scattering (SERS) substrates were systematically determined. The sizes of the prepared silver nanoparticles were identified in TEM images, which were 31 ± 5 nm and almost all of them were aggregated in three or four particles in solution. The optimum condition was determined by relative enhancement of the SERS signal in the spectra of benzoic acid. The observed SERS signals in the prepared solution were remarkably reproducible and the solution was stable for a week at least. In addition, spectra of biphenyl derivatives adsorbed on silver nanoparticles have been measured by SERS. Assignments for the vibrational peaks observed in the SERS spectra have been performed utilizing density functional theory (DFT) calculations. Based on excellent agreement between the experimental and the calculated results achieved, structures of 4,4'-biphenyl dicarboxylic acid (BPDC), 4,4'-biphenyldithiol (BPDT), 4,4'-bis(mercaptomethyl) biphenyl (BMBP) on silver were defined their adsorption behaviors were also characterized.

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발표코드: **PHYS.O-11**

발표분야: General Oral Presentation

발표종류: 구두발표, 발표일시: 금 12:10, 좌장: 권오훈

Vibronic emission spectroscopy of benzyl-type radicals: Jet-cooled 2-fluoro-5-chlorobenzyl radical

윤영욱 채상열[1] 이상국[*]

부산대학교 화학과 [1](주)엔지텍 연구개발팀

Vibronically excited but jet-cooled benzyl-type radicals were generated from the precursor 2-fluoro-5-chlorotoluene using a pinhole-type glass nozzle designed for supersonic jet expansion along with corona discharge, from which the visible vibronic emission spectrum was recorded from the discharge system with a long-path monochromator. The spectrum shows a complicate vibronic pattern of two benzyl-type radicals; 2-fluoro-5-benzyl and 2-fluorobenzyl radicals. From an analysis of the spectrum observed, we identified the formation of two benzyl-type radicals, 2-fluoro-5-benzyl and 2-fluorobenzyl radicals in the corona discharge of precursor, and determined for the first time the electronic energy in the $D_1 \rightarrow D_0$ transition and vibrational mode frequencies in the D_0 state for both benzyl-type radicals.

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발표분야: General Oral Presentation
발표종류: 구두발표, 발표일시: 금 12:20, 좌장: 권오훈

Effects of Entanglements of Polymers on the Dynamics of a Carbon Nanotube in Polymeric Materials

김민정 성봉준*

서강대학교 화학과

Carbon Nanotube/Polymer nanocomposites have been investigated extensively due to their potential applicability in many areas. When a sufficient amount of carbon nanotubes (CNTs) are inserted in polymeric matrices, the mechanical strength of composites increases sharply due to the entanglement of polymers around the CNTs. However, there have been few studies at a molecular level on how such an entanglement would affect the dynamics of CNTs and polymers, and enhance the mechanical strength. Therefore, we employ molecular dynamics simulations to investigate the effects of entanglement. We estimate the winding number of polymers around a CNT to quantify the degree of entanglements. Not surprisingly, the winding number increases with the degree of polymerization of polymers. However, we find that the rotational dynamics decouple from the translational dynamics, i.e., the rotational diffusion of CNTs decreases quickly with the stiffness of CNTs while the translational diffusion of CNTs hardly changes with the stiffness. More interestingly, the translational diffusion of CNTs becomes anisotropic depending on the direction with respect to the molecular axis. We discuss such an interesting dynamic phenomena based on the winding number, i.e., the entanglement effects.

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발표분야: General Oral Presentation
발표종류: 구두발표, 발표일시: 금 12:30, 좌장: 권오훈

Novel analysis of steady-state mRNA expression reveals hidden oscillatory feature of transcription rate fluctuation

박성준 임유림 양길석 김지현* 성재영*

중앙대학교 화학과

We present a novel theoretical model for description of the cell-to-cell variation of mRNA level among isogenic cells. When the promoter of a probe gene is turned on, the previous models have assumed a constant transcription rate while the present model considers the transcription rate in the active promoter state a stochastic variable that fluctuates not only over time but also over cell. It is shown that the fluctuation in transcription rate is an essential ingredient required to explain the fluctuation in mRNA copy number at high mRNA expression levels. Furthermore, We could extract a short-time profile of transcription rate autocorrelation function from the experimental data of steady-state mRNA expressions on the basis of our analytic formula and found that the resulting correlation function shows an oscillatory feature. In terms of time-dependent standard deviation of mRNA copynumber, which is closely related to the rate autocorrelation function, it is found from stochastic simulation consisting of RNA polymerase (RNAP)-promoter binding, successful initiation, and elongation that such an oscillatory behavior can be produced when the distribution of time required for successful initiation completion has a highly sub-Poisson character, leading to a well-seperated sequential alignment of RNAPs on a single gene. The present theory provides a unified description linking the steady-state mRNA statistics to the underlying microscopic dynamics of transcription rate, the oscillatory feature of which is consistent with various experimental observations.

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Studying Abnormality in Density Functional Theory

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연세대학교 화학과 [1]Department of Chemistry, University of California, Irvine

In this presentation, we introduce a general way to classify and reduce errors in density functional calculations. For any self-consistent Kohn-Sham density functional theory (KS-DFT), the total energy error can be separated to contribution due to the approximate functional and that due to the approximate density. Usually, the functional error dominates, but in many interesting situations, the density-driven error dominates. We show examples of these ‘abnormal’ calculations with large density-driven error, including electron affinities, dissociation of molecules into charged fragments, transition state barriers, and ions and radicals in solution. By using a more accurate density, error can be significantly reduced in these abnormal calculations. We provide a practical way to distinguish an abnormal KS-DFT calculation, where small energy gap between HOMO and LUMO may indicate a substantial density-driven error. Finally, we suggest a simple and practical method to reduce the density-driven error in abnormal cases by evaluating DFT energy upon Hartree-Fock(HF) density (HF-DFT).

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발표코드: **PHYS.O-15**

발표분야: General Oral Presentation

발표종류: 구두발표, 발표일시: 금 12:50, 좌장: 권오훈

Elastic and Electronic Properties of π-Conjugated Nickel Bis(dithiolene) Complex Nanosheet

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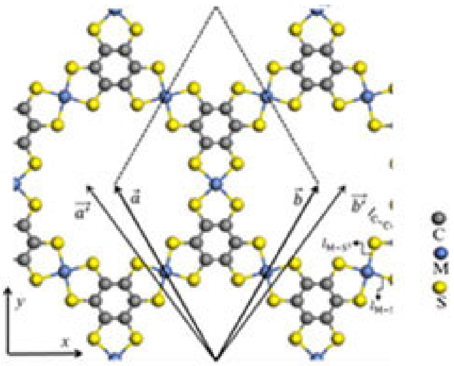
전주대학교 나노신소재공학과 [1]전북대학교 화학과

Using the first-principles calculations, we have investigated elastic and electronic properties of two-dimensional (2D) π-Conjugated M-Bis(dithiolene) Nanosheet (M-C4S4) (M= Ni, Pd), between which the NiC4S4 sheet was recently synthesized. Under isotropic strain, our calculation of the in-plane stiffness parameter C and Poisson ratio indicates that the 2D M-C4S4 are even softer than grapyne-4, which is the most porous among all graphyne analogs considered. At a critical tension of 13%, the M-sulfur (M-S) bond length becomes so large that both sheets become fragmented. At 6% strain, the NiC4S4 sheet changes from a semiconductor into a semimetal. On the one hand, the PdC4S4 sheet remains metallic irrespective of the magnitude of the strain, even at zero strain. Our delated band structure analysis shows that these observation can be ascribed to a charge transfer from the M ion to the sheet and as well as to the weakening of covalent bonds under the strain. Under an uniaxial strain of 24% along the X axis, a nonreversible structural change occurs due to a partial breaking of a specific M-S bond, while both sheets undergo fragmentation at 18% strain along the Y axis. This observation can be understood in terms of the number of underlying M-S bonds. Based on the band structure analysis, we will also discuss the change of the electronic structure under each of the uniaxial strains.


a'
a
b
b'
l_{C-C}
l_{M-S}
C
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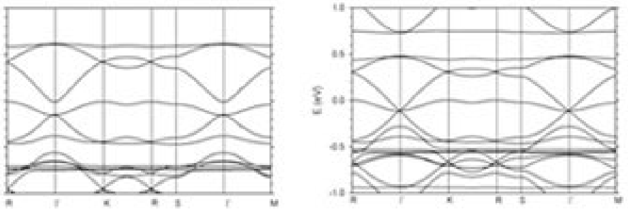
1.0
0.5
0.0
-0.5
-1.0
E (eV)
R
Γ
K
R
S
Γ
M

일시: 2014년 4월 16~18일(수~금) 3일간

장소: 일산KINTEX

발표코드: **ANAL.O-1**

발표분야: Oral Presentation of Young Analytical Chemists

발표종류: 구두발표, 발표일시: 금 10:00, 좌장: 이승호

Electrochemical analysis of anion substituted olivine materials for Li rechargeable battery

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울산대학교 화학과

There has been considerable interest in olivine structure as a cathode active material for Li rechargeable battery due to its strong phosphorus-oxygen covalent bond and excellent stability. The anion substituted $LiFe_{0.4}Mn_{0.6}PO_4$ materials have been synthesized by solid state reaction using planetary mill method without additional carbon source. The XRD, MAS NMR and XPS results of composite indicate anions have been completely substituted to PO4 sites without structural modification. Electrochemical analysis has been performed with various C-rates, and initial discharge capacity of over 130 mAh/g at 0.1 C rate for $LiFe_{0.4}Mn_{0.6}(PO_4)_{0.99}F_{0.03}$ has obtained.

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장소: 일산KINTEX

발표코드: **ANAL.O-2**

발표분야: Oral Presentation of Young Analytical Chemists

발표종류: 구두발표, 발표일시: 금 10:20, 좌장: 이승호

Exploring an optimal temperature providing improved spectral specificity of complex samples and enhancing accuracy of quantitative analysis

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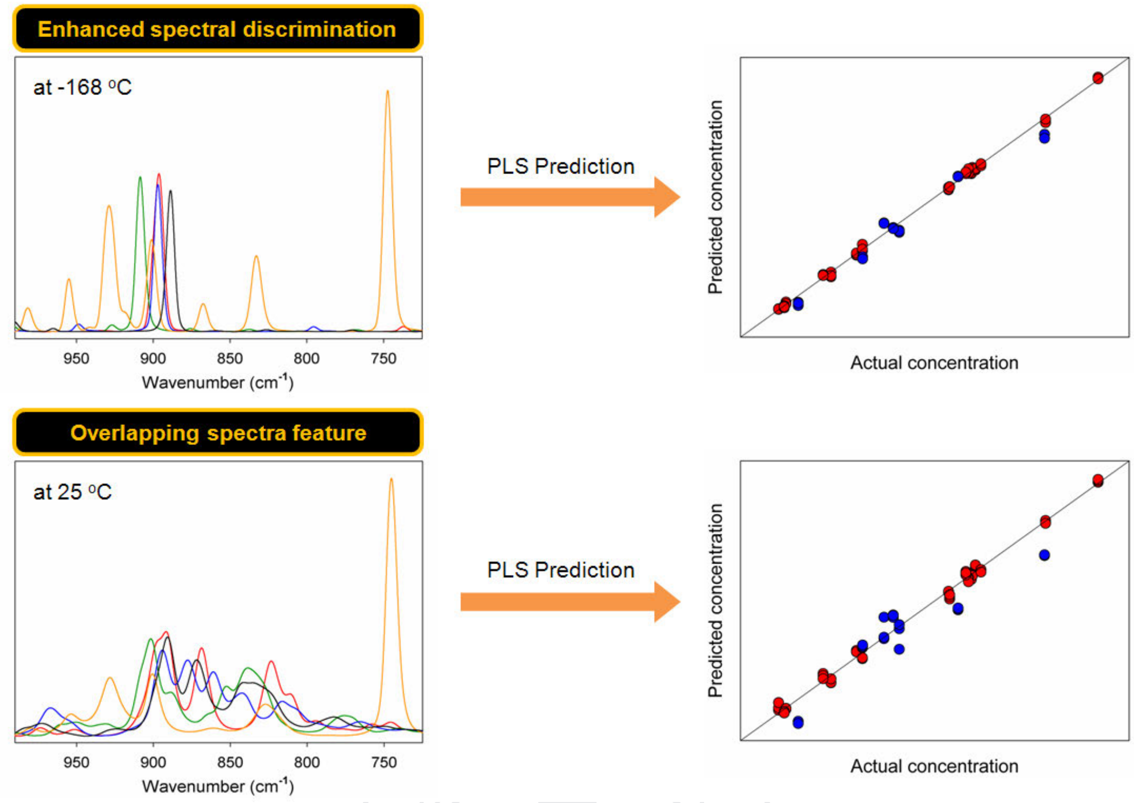
한양대학교 화학과

When compositional analysis for complex mixture samples is conducted using spectroscopic methods combined with multivariate data analysis, the spectral selectivity is usually an important concern since resulting spectral feature will be highly overlapped each other. Any analytical methods that can improve the spectral selectivity would be beneficial to possibly enhance the accuracy of compositional analysis. In this study, we have investigated the variation of Raman spectral bands of synthetic hydrocarbon mixtures that were composed of eleven hydrocarbons (*n*-hexane, *n*-heptane, *n*-octane, *n*-nonane, isooctane, cyclohexane, methylcyclohexane, benzene, toluene, xylene and indan) when these were measured in a frozen state at low temperatures. By changing the sample temperature from cryogenic to near room temperature, Raman spectra were periodically collected. The variations in bandwidth, band position as well as relative band intensity were clearly observed. The most dominant variation was observed for linear hydrocarbons such as *n*-hexane, *n*-heptane, *n*-octane and *n*-nonane. Since *n*-paraffins are easily compressible and deformable in frozen conditions, the subsequent spectral variations could be diverse depending on their molecular structures. Using the spectra collected at each period, partial least squares (PLS) regression was used to determine the concentrations of each component. The variation of PLS accuracies according to temperature variation was finally examined and relevant justification was provided the improved accuracy.


Enhanced spectral discrimination
at -168 °C
950
900
850
800
750
Wavenumber (cm-1)
PLS Prediction
Predicted concentration
Actual concentration
Overlapping spectra feature
at 25 °C
950
900
850
800
750
Wavenumber (cm-1)
PLS Prediction
Predicted concentration
Actual concentration

일시: 2014년 4월 16~18일(수~금) 3일간

장소: 일산KINTEX

발표코드: **ANAL.O-3**

발표분야: Oral Presentation of Young Analytical Chemists

발표종류: 구두발표, 발표일시: 금 10:40, 좌장: 이승호

Study on antidiabetic activity of wheat and barley using asymmetrical flow field-flow fractionation coupled with multiangle light scattering

DouHaiyang 이승호*

한남대학교 화학과

The capacity of asymmetrical flow field-flow fractionation (AF4) coupled online with multiangle light scattering (MALS) and refractive index detector (RI) (AF4-MALS-RI) for monitoring of change in molecular conformation of wheat and barley during germination process was evaluated. AF4 provides separation of biomacromolecules based on their hydrodynamic sizes, and MALS yields the molar mass and molecular size (radius of gyration, R_g). In vitro and in vivo anti-hyperglycemic effect of germinated wheat and barley was studied. The relationship between antidiabetic activity and molecular conformation was, for the first time, investigated. The ratio of R_g to the hydrodynamic radius (R_h) and the apparent density were proven to be important parameters as they offer an insight into molecular conformation. Results showed that, when geminated, the apparent density and the antidiabetic activity of barley were significantly increased, suggesting germination makes the molecules more compact which could contribute to enhancement of their antidiabetic activity. The information obtained by AF4-MALS-RI is valuable for understanding of germination mechanism, and thus for developing functional foods.

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Absolute quantification of plasmid DNA using high sensitivity flow cytometry

유희봉 박상열[1,*]

과학기술연합대학원대학교(UST) 생물분석과학 [1]한국표준과학연구원(KRISS) 바이오임상표준센터

This work demonstrates accurate measurement of the concentration of low-level plasmid DNA by counting individual DNA molecules using a high-sensitivity flow cytometric setup. Plasmid DNA is a widely used form of DNA, and its quantity often needs to be accurately determined. This work establishes a reference analytical method for direct quantification of low-level plasmid DNA molecules prepared as reference standards for polymerase chain reaction-based DNA quantification. The model plasmid DNA pBR322 (4.58 kbp) was stained with a fluorescent dye and was detected on a flow stream in a micro-fluidic channel with laser-induced fluorescence detection, for which the DNA flow was electro-hydrodynamically focused at the center of the channel. 200?8,000 DNA particles in a ~1 μL sample volume were counted within 2 minutes in an ‘exhaustive counting’ manner, which facilitated quantitation without calibration. The sample volume was measured and validated from the close agreement of the results of two independent measurement methods. Within the given concentration range, an excellent measurement linearity (R = 0.999) was achieved with appropriate data processing for simultaneous exposures of DNA to the detector. The validity of the proposed method was confirmed from the close agreement with the results of quantitation of enzymatically released nucleotides using capillary electrophoresis.

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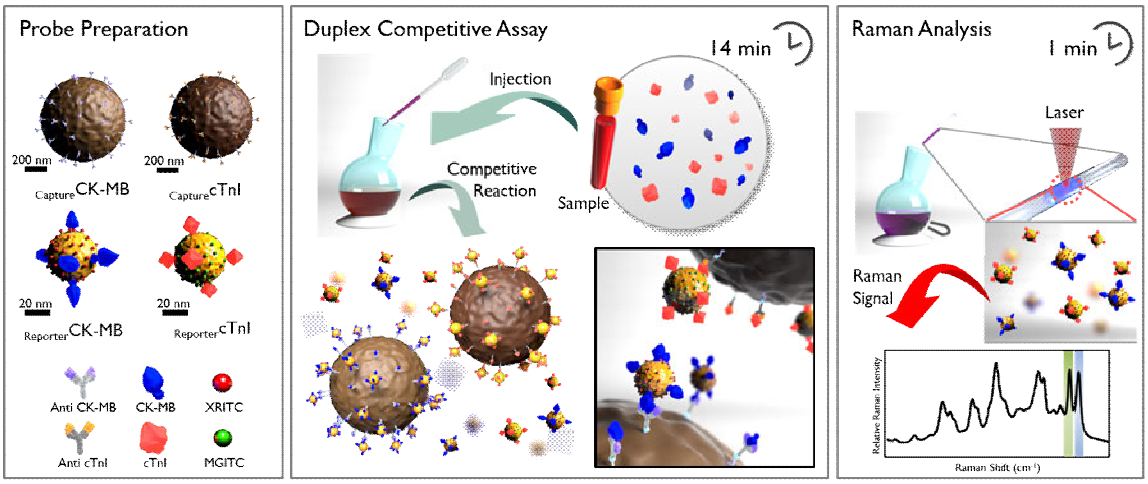
Simultaneous Detection of CK-MB and Troponin I Markers Using SERS-based Competitive Immunoassay

전향아 이상엽[1] 주재범[1,*]

한양대학교 바이오나노공학과 [1]한양대학교 생명나노공학과

There have been compelling evidences that the early diagnosis of acute myocardial infarction (AMI) involves the determination of the serum levels of a group of cardiac biomarkers. Among the most frequently used biomarkers, the simultaneous estimation of CK-MB and cTnI marker levels in blood, shortly after the AMI incidence, greatly contributes to the clinical applicability for the early diagnosis of AMI. Herein, we demonstrate a SERS-based competitive immunoassay for simultaneous determination of CK-MB and cTnI. The competitive assay requires no sample processing, beyond centrifugation or filtration to remove particulates, and is significantly less sensitive to sample dilution and sample matrix effects than the sandwich immunoassay format. Therefore, it provides much tighter data with lower variability between duplicate samples and lower variability between assays. Furthermore, the competitive assay requires a shorter detection time than the sandwich immunoassay because only one binding process between antigen and antibody is needed. Using this SERS-based competitive assay technique, the simultaneous detection of CK-MB and cTnI cardiac markers in blood serum was achieved under a single excitation wavelength. This novel immunoassay has multiple advantages including a quick assay time (less than 15 min), a non-washing step (just magnetic beads separation), and simultaneous multiple marker detection using reliable, sharp, and easily distinguishable SERS peaks.


Probe Preparation
200 nm
200 nm
Capture CK-MB
Capture cTnI
20 nm
20 nm
Reporter CK-MB
Reporter cTnI
Anti CK-MB
CK-MB
XRITC
Anti cTnI
cTnI
MGITC
Duplex Competitive Assay
14 min
Injection
Competitive Reaction
Sample
Raman Analysis
1 min
Laser
Raman Signal
Relative Raman Intensity
Raman Shift (cm⁻¹)

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셀룰로스 유도체(HPMC & HEMC)의 레올로지 분석을 이용한 Gel strength와 Thermal gelation 연구

송민주

삼성정밀화학(주) 그린소재개발팀

셀룰로스 유도체 중 Hydroxypropylmethylcellulose(이하 HPMC)와 Hydroxyethylmethylcellulose(이하 HEMC)는 수용성 고분자로 식품, 의약품, 건축용, 페인트, 생활용품등 다양한 분야에서 활용된다. 각 용도별로 많이 사용되는 치환체와 치환도가 있으며 치환도와 점도 입도, 열적거동 등 이 응용물성에서 해당 고분자를 선택하는 기준이 된다. 점도와 입도등 기초 물성이 동일할 때, 구조적인 측면에서 접근 하여 합성법에 따라 치환도 및 치환패턴이 달라지며 이로인해 응용 물성에 영향을 주는 경우가 있다. 본 연구에서는 레오미터를 이용하여 수용성 고분자들의 용액 상태에서의 Gel strength 와 Thermal gelation 거동을 관찰하고 결과를 이용하여 적용 분야와 범위를 선정할 때 활용 하고자 한다.

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발표분야: Oral Presentation of Young Biochemists
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Harnessing the destructive power: Activity regulation of a bacterial heat-shock protease, DegP

김석희

서울대학교 화학부

Proper elimination of misfolded proteins is essential for cellular life because they are often toxic to cells. Proteases in protein quality control (PQC) remove misfolded proteins by degradation, but they are double-edged swords because uncontrolled proteolysis can be wasteful or cytotoxic. How the PQC proteases regulate their activity in different environments remains to be determined. DegP is the major PQC protease in the bacterial periplasm, and belongs to the highly conserved HtrA family, whose members are associated with bacterial pathogenesis and human diseases. Here I present that distinct self-regulatory elements in architecture control DegP proteolysis and maintain the cellular fitness during misfolded protein stress in vivo. Biochemical, biophysical, and structural studies revealed mechanisms of activity regulation in vitro; the bipartite mode of substrate binding, dynamic conversion between inactive and active states, and assembly of large cages. Mutations that modify these processes could generate a rogue protease that kills cells by disrupting essential cellular processes in periplasm and this lethality could be suppressed by a mutant lipoprotein functioning as a novel inhibitor or new intragenic mutations that offset the effect of the original mutation. These results demonstrate that there is a delicate balance of quality control proteolysis in bacterial periplasm, and suggest that its disruption either by inhibition or activation may be a good strategy for antibiotic development.

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A novel deoxysugar hydroxylase KdoO and its characterization

정학숙

한국과학기술연구원(KIST) 의공학연구소/테라그노시스연구단

As a part of lipopolysaccharide (LPS) several Gram-negative pathogens such as Yersinia pestis, Burkholderia cepacia, and Acinetobacter haemolyticus, synthesize an isosteric analog of 3-deoxy-D-manno-oct-2-ulosonic acid (Kdo), known as D-glycero-D-talo-oct-2-ulosonic acid (Ko), in which the axial hydrogen atom at the Kdo 3-position is replaced with OH. A novel Fe2+/?-ketoglutarate/O2-dependent dioxygenase, Kdo 3-hydroxylase (KdoO) converts Kdo to Ko and is the first example of a sequenced deoxy-sugar hydroxylase reported so far. Fe(II)/O2/a-ketoglutarate dependent dioxygenases play important roles in a variety of oxidative transformations in different biological pathways; DNA repair (AlkB), O2 sensing mechanism in human (HIF-hydroxylases, PHDs), histone demethylation (PHF8), and taurine catabolism (TauD) as well as herbicide degradations (RdpA and SdpA). While this class enzymes share a key catalytic mechanism, their sequence similarities are very low. Homologues of KdoO are found exclusively in Gram-negative bacteria, including the human pathogens Burkholderia mallei, Yersinia pestis, Klebsiella pneumoniae, Legionella longbeachae, Coxiella burnetii, and the plant pathogen Ralstonia solanacearum. Biochemical studies and high resolution complex structures obtained not only serve as a model to study mechanisms of this enzyme family but also provide a unique data set to study differences of transition metal coordination in metal/protein complexes.

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발표분야: Oral Presentation of Young Biochemists

발표종류: 구두발표, 발표일시: 금 10:50, 좌장: 최수혁

Multiplex Protein Detection by Using Optically Encoded Microbeads

전봉현

건국대학교 생명공학과

Since protein detection has potential for early detection and diagnosis of various diseases, there have been considerable interests in the development of multiplex protein detection techniques. Among the various techniques for high-throughput protein screening, optically encoded beads combined with fluorescence-based target monitoring have great advantages over planar array-based multiplexing assays. Recently, our group has developed several kinds of optical encoded beads such as multilayer fluorescence beads and SERS encoded beads for generating a large number of coding. Moreover, their beads based novel protein detection strategies which can be applied for label-free protein detection were also developed. We will discuss these optically encoded beads and multiplex detection systems.

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CaV1.3-selective L-type calcium channel antagonists: potential new therapeutics for Parkinson's disease

Soosung Kang Gary Cooper Dalton Surmeier Richard Silverman*

Northwestern University

Cav1.3 L-type calcium channels (LTCCs) engagement in autonomous pacemaking of substantia nigra pars compacta (SNc) dopamine (DA) neurons renders SNc DA neurons selectively vulnerable in animal models of Parkinson's disease (PD). This selective vulnerability is manifested as Cav1.3-dependent phasic dendritic calcium oscillations and mitochondrial oxidant stress. LTCCs expressed in the brain are heterogeneous. The predominant class of LTCC has a CaV1.2 pore-forming subunit. LTCCs with a CaV1.3 pore-forming subunit are much less abundant. Thus, selectively antagonizing CaV1.3 could provide a means of diminishing cell loss in PD without producing side effects accompanying general antagonism of LTCCs. We performed high-throughput screening of diverse chemical libraries and identified pyrimidine-2,4,6-triones as a potential scaffold; SAR-based modification of this scaffold led to 1-(3-chlorophenethyl)-3-cyclopentylpyrimidine-2,4,6-(1H,3H,5H)-trione (SKP004C08), a potent and highly selective CaV1.3 antagonist. We show that SKP004C08 inhibition is selective for Cav1.3 in acutely dissociated adult SNc DA neurons. We also demonstrate that inhibition of Cav1.3 in adult SNc DA neurons in acute brain slices can attenuate dendritic calcium oscillations and reduce mitochondrial oxidant stress without changes in pacemaking. Thus, SKP004C08 offers a novel and improved potential therapeutic option in reducing selective vulnerability of SNc DA neurons in PD via Cav1.3 selective inhibition.

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발표분야: Oral Presentation of Young Biochemists

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Computational Design of Supramolecular Protein Assemblies

김용호

성균관대학교 자연과학대학/화학과, 성균나노과학기술

Over the last two decades, newly emerging nanomaterials have demonstrated a great potential to overcome limitations in current engineering technology. However, site-specific assembly of nanomaterials for highly integrated systems still remains as a major challenge. De novo protein design has been historically used to validate the principles governing the process of biomolecular folding and assembly. However, de novo design of proteins and peptides from physical principles may have an even greater impact when applied to recognizing and organizing nanomaterials. We demonstrate that nano-bio hybrid structures can be engineered to assemble in a structurally-specific manner, and this presents a promising way of addressing current limitations in nanoscale assembly. Here, I will introduce protein-design based on computational modeling to successfully engineer a series of hybrid structures composed of carbon-based nanomaterials and artificial proteins. In addition, this talk will describe general rules for designing peptides that recognize surface lattices and further self-associate to achieve superstructure with major progress in the field of nano-assembly.

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발표분야: Oral Presentation of Young Biochemists
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Detergent design for membrane protein study

채필석

한양대학교 생명나노공학과

Membrane proteins play central roles in a variety of cellular functions such as signal transduction and material transfer across membrane barrier. These bio-macromolecules tend to denature or aggregate when solubilized with conventional detergents from the native membranes for the studies. This protein degradation occurring in detergent micelles is likely due to the limited utility of these membrane-mimetic agents, necessitating developments of novel agents with enhanced efficacy. Detergent structure-property relationships are essential in these efforts. Despite a large number of detergent studies, however, little information regarding these relationships is available. In the current presentation, we will discuss about some of these relationships, based on the results of several classes of novel amphiphiles. These detergent structure-property relationships will facilitate the development of promising amphiphiles, thereby leading to advances in membrane protein research.

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발표분야: Oral Presentation for Young Organic Chemists
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Dynamic Supramolecules by Self-Assembly of Rigid-Flexible Amphiphiles: Rational Designs and Their Application to the Chemical Reaction

김용주 이명수*

Jilin University

Extensive investigations on the self-assembly behavior of synthetic amphiphiles have created well-defined shapes and sizes including vesicles, spherical micelles, cylindrical micelles, tubes, ribbons, bilayers, helices, networks, and toroids. The molecular assembly of the amphiphilic molecules through weak noncovalent is ideally suitable for the construction of the responsive materials since the dynamic and reversible conformational changes can be triggered by external environments. Among a variety of self-assembling building blocks, rigid-flexible block molecules which are composed of rigid rod and flexible coil segments are excellent candidates for creating well-defined supramolecular structures in selective solvents for flexible side chains. Herein, the guest molecule responsive nanosheets and the thermodynamic nanotubules that have open-close motion will be introduced including the rational design of molecules and the efficient synthetic method. In addition, these nanostructures will be applied as catalyst for organic reaction.

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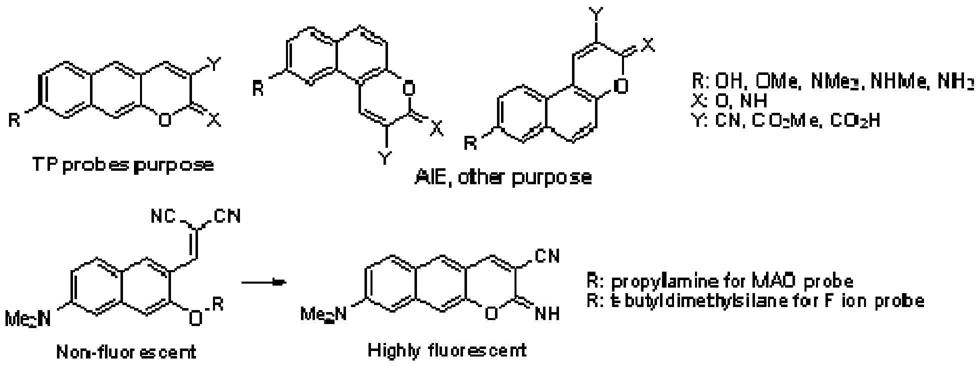
발표분야: Oral Presentation for Young Organic Chemists
발표종류: 구두발표, 발표일시: 금 10:15, 좌장: 조천규

Development of New Two-photon Absorbing Materials and Fluorescent Probes: Linear and Bent Type Pi-Extended Coumarin Derivatives

김도경 안교한*

포항공과대학교 화학과

Two-photon (excitation) microscopy (TPM) combined with the laser excitation technology has arrested recent attention in the bioimaging area because it shows several advantageous features over one-photon excitation microscopy (OPM). TPM is most often emphasized to be “less photo-toxic, less photo-bleaching and less photo-damaging”. In addition, TPM enables deeper tissue (700-1100 nm) imaging with high spatio-temporal resolution, and thus is particularly useful for tissue imaging where auto-fluorescence becomes serious in the case of OPM.The primary aim of this research is to develop new two-photon materials which show desirable photo-physical properties for bioimaging, overcoming some drawbacks of known dyes such as acedan and coumarin derivatives. This research is also focused on the studies of new platforms for the development of two-photon fluorescent probes for biologically important analytes, based on the reaction-based sensing approach. As a results, we have developed novel π-extended coumarin dyes, which show very promising properties as two-photon excitable dyes and also molecular shape-dependent luminescent behaviours.#Ref: (a) Kim, Kim, D.; Sambasivan. S.; Nam. H.; Kim. K. H.; Kim. J. Y.; Joo. T.; Lee. K.; Kim. K.; Ahn. K. H. Chem. Commun. 2012, 48, 6833. (b) Kim, I,; Kim, D.; Ahn. K. H. Asian J. Org. Chem. 2012, 1, 60.


TP probes purpose
AIE, other purpose
R: OH, OMe, NMe2, NHMe, NH2
X: O, NH
Y: CN, CO2Me, CO2H
NC
CN
Me2N
O
R
Non-fluorescent
CN
NH
Highly fluorescent
R: propylamine for MAO probe
R: t-butyldimethylsilane for F ion probe

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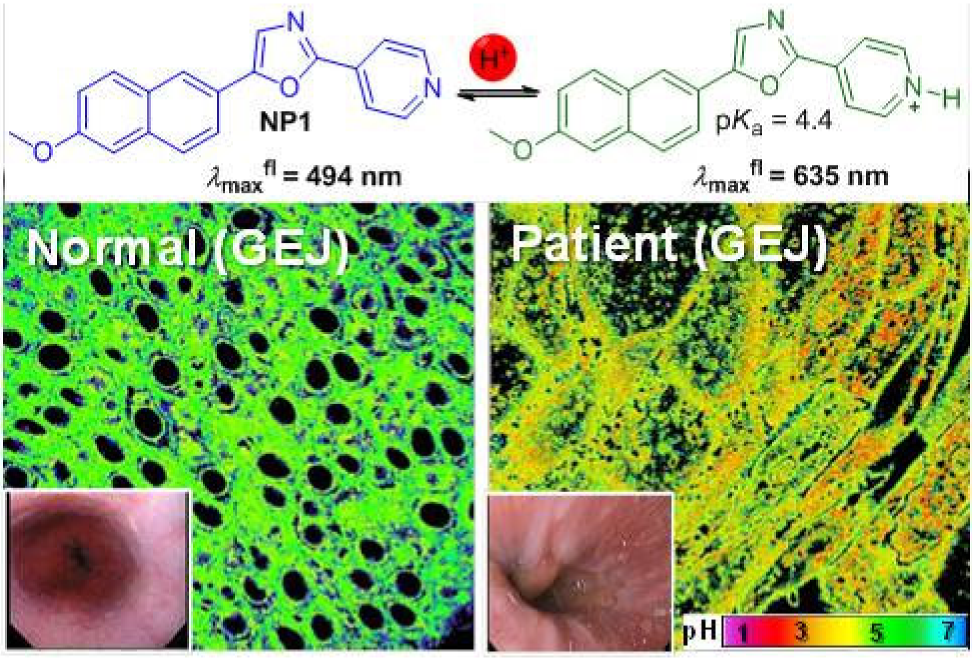
Biomedical applications with two-photon fluorescence probes

임창수 조봉래*

고려대학교 화학과

Optical imaging with fluorescence microscopy is a vital tool in the study of living systems. The most common method for cell imaging is confocal microscopy, which utilizes the fluorescence emitted from probe-labeled cells, by excitation with a single UV-Vis photon.[1]Two-photon microscopy (TPM), which uses two-photons of lower energy as the excitation source, is a vital tool in biology and clinical science, due to its capacity to image deep inside intact tissues for a long period of time. To make TPM a more versatile tool in biomedical research, we have developed a variety of two-photon probes for specific applications. In this mini review, we will briefly discuss two-photon probes for lipid rafts, lysosomes, mitochondria, and pH, and their biomedical applications.[2]Reference1. Pawley, J. B. (2006) Handbook of biological confocal microscopy. 3rd ed. Springer, Berlin, Germany.2. Lim, C. S. and Cho, B. R. *BMB Reports*. 2013, 46, 188-194.


NP1
λ_{max}^{fl} = 494 nm
H+
pK_a = 4.4
λ_{max}^{fl} = 635 nm
Normal (GEJ)
Patient (GEJ)
pH 1 3 5 7

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Catalytic Acylation of Inactive C-H Bonds via C-H Bond Activation

박지혜

성균관대학교 약학과

The development of new carbon-carbon bond-forming reactions continues to be an essential goal in organic chemistry. Traditional metal-catalyzed cross-coupling reactions between aryl metal reagents and aryl halides are well-established methods for the construction of C?C bonds and synthesis of complex molecules. Recently, transition-metal-catalyzed decarboxylative cross-coupling reactions using aryl carboxylic acids as aryl surrogates have received much attention since such transformations provide new opportunities to use readily available carboxylic acids as starting materials for organic synthesis. Transition-metal-catalyzed oxidative acylation of sp^2 C?H bonds in aromatic compounds with various directing groups, e.g., pyridines, oximes, acetanilides, and indole, with aldehydes or alcohols were reported. However, decarboxylative C?H bond acylations using α-oxocarboxylic acids as acyl surrogates were relatively unexplored. Goossen first demonstrated a palladium-catalyzed decarboxylative crosscoupling reaction of aryl bromides with α-keto carboxylate salts as acyl anion equivalents to afford diaryl ketones. Ge described elegant studies on a palladium-catalyzed decarboxylative acylation of acetanilides and phenylpyridines with α-oxocarboxylic acids as acyl sources via C?H bond activation. Recently, Guo and Duan described a decarboxylative acylation of cyclic enamides with α-oxocarboxylic acids to provide β-acyl enamides. Herein we described our recent result on a Pd-catalyzed decarboxylative *ortho*-acylation of *O*-methyl ketoximes and phenylacetamides with α-keto acids via C?H bond activation. This protocol provides an efficient access to a range of ortho-acyl phenylacetamides, which can be easily converted to 3-isochromanone derivatives.

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발표코드: **ORGN.O-5**

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Synthesis of Pyrroles from Terminal Alkynes, *N*-Sulfonyl Azides, and Alkenyl Alkyl Ethers through 1-Sulfonyl-1,2,3-triazoles

김철의 이필호*

강원대학교 화학과

Pyrroles are significant structural motifs found not only in valuable bioactive molecules but also in a massive range of natural products. They also find broad applications in supramolecular chemistry and materials science as conjugated polymers. The metal carbene species have inherently electrophilic character, they can react with a wide range of nucleophiles. On the contrary, the nitrogen atom of the α-imino group is nucleophilic in nature to react with various electrophiles. We have reported the synthetic method of substituted pyrroles from the transannulation of α-imino rhodium carbenes generated in situ from 1-sulfonyl-1,2,3-triazoles with a wide reage of alkenyl alkyl ethers followed by elimination reaction. Moreover, it has been also demonstrated that pyrroles can be prepared from terminal alkynes, tosyl azide, and alkenyl alkyl ethers through a one-pot sequential reaction.

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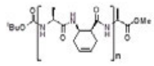
발표분야: Oral Presentation for Young Organic Chemists
발표종류: 구두발표, 발표일시: 금 11:15, 좌장: 조천규

2-Aminocyclohex-4-enecarboxylic Acid as a New Building Block of Helical Foldamers

권선미 강필재 최수혁*

연세대학교 화학과

1:1 α/β-peptides containing cyclic β-amino acid have a specific conformation ("foldamer").[1] We used the cyclic β-amino acids for building blocks, which can form the divers helix and stable secondary structure with α-amino acids by intramolecular hydrogen bonding. The six-membered cyclic β-amino acids can be obtained from cyclohexadiene by addition of chlorosulfonyl isocyanate.[2] We analyzed our oligomers (Fig 1) using 1H-NMR, IR, CD and X-ray crystallography analysis. IR spectrum (in 1 mM dichloromethane, Figure 2a) shows the existence of intramolecular hydrogen bond at 3344 cm-1 in the N-H stretch region and CD spectrum (in 0.1 mM acetonitrile, Figure 2b) of 1:1 α/β-peptides displays a characteristic 11/9 helical intensity at 198 nm and 224 nm. These results mean that our 1:1 α/β-peptides can form stable secondary structures. Using X-ray crystallography analysis, we finally confirm our oligomers adopt stable 11/9 helix. (Figure3)References1. Samuel H. Gellman, “Foldamers: A Manifesto”, Accounts of Chemical Research, Vol. 31, No. 4, (1998), 173-1802. Eniko3 Forro, Judit A´ rva and Ferenc Fu¨ lo¨p* Tetrahedron: Asymmetry, Vol. 12, (2001) 643?649



1, n=1
2, n=2
3, n=3

Fig 1. 1:1 α/β-peptide oligomers

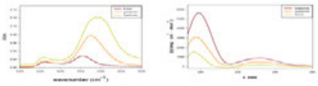


Figure 2. a) IR and b) CD spectrum for oligomers

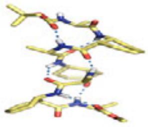


Figure 3. molecular drawing of heptamer

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발표종류: 구두발표, 발표일시: 금 11:30, 좌장: 조천규

Metal-Free Protodeboronation of Electron-Rich Arene Boronic Acids and Its Application to ortho-Functionalization of Electron-Rich Arenes Using a Boronic Acids as a Blocking Group

안수진 이춘영 천철홍*

고려대학교 화학과

Boronic acids are one of the most useful intermediates due to their low toxicity, stability, and ready availability. Although some boronic acids, particularly heteroaromatic boronic acids, are known to unstable, many arene boronic acids are generally believed to be stable and, thus, more than 9000 phenyl boronic acid derivatives are currently commercially available. In contrast to the general belief on the stability of boronic acids, there have been few studies on the actual stability on the boronic acids, and some of the boronic acids, in particular, electron rich arene boronic acids, are not stable even though they are commercially available. For example, we recently found that ortho-and para-phenol boronic acids readily underwent metal-free thermal protodeboronation in wet DMSO, which renders it difficult to store these important boronic acids. With this rather unusual metal-free thermal protodeboronation of phenol boronic acids, we were curious whether this type of metal-free protodeboronation might be the general behaviours of not only phenol boronic acids but also electron-rich boronic acids. Thus, we investigated metal-free thermal protodeboronation of electron-rich arene boronic acids including various reaction parameters to affect the metal-free protodeboronation, such as solvent, electron-density on the arene ring system, acidity of proton source, and Lewis acidity of boron atom in the boronic acid. Based on these results, we established the reaction conditions where the boronic acid functionality could be movable and proposed the reaction mechanism for this protodeboronation. Furthermore, a novel method for the ortho-functionalization of electron-rich arenes has been developed using the boronic acid moiety as a blocking group and subsequent protodeboronation.

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발표분야: Oral Presentation for Young Medicinal Chemists

발표종류: 구두발표, 발표일시: 금 10:00, 좌장: 임환정

Strategy for Chemical Library Design for Drug Discovery

최인희

한국파스퇴르연구소 의약생유기화학

Finding a right hit compound from high throughput screening (HTS) which will be optimized to a drug candidate is not a simple task. Currently, a very high and expensive failure rate in finding the reasonable lead series from HTS during the early-stage drug discovery is a bottleneck in drug development. Therefore, selecting meaningful compounds from a slew of commercially available compounds is important. Not only the number of compounds and structural diversity but also druglike physicochemical properties are the key factors in constructing library. IPK has established chemical libraries sensitively to encompass these diversity and physicochemical property aspects. Compounds from validated chemical vendors were curated in the first place. In order to select drug-like compounds, a combination of Lipinski’s, Veber’s and Oprea’s rules were applied. Also, compounds having non-drug like fragments or toxicophores were filtered. To obtain structural diversity, lead-like Bemis-Murcko substructures were generated and compounds with those similar substructures were not cherry picked among chemical libraries. Combining lead-likeness factor which is complement to drug-likeness factor contributed to the good quality of chemical libraries. A small chemical found as a hit compound from HTS screening was successfully optimized as the first-in-class TB drug candidate, Q203.

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발표분야: Oral Presentation for Young Medicinal Chemists
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Solid-phase Synthesis of 2-Amino/amido-1,3,4-oxadiazole and 1,3,4-thiadiazole Derivatives via Reagent-based Cycilzation of Thiosemicarbazide Intermediate Resin

양승주 공영대*

동국대학교 화학과

A 2-amino/amido-1,3,4-oxadiazole and 1,3,4-thiadiazole library has been constructed as a Canonical Wnt signaling pathway inhibitor by solid-phase organic synthesis. The key step on this solid-phase synthesis involves the preparation of polymer-bound 2-amino-1,3,4-oxadiazole and 1,3,4-thiadiazole resin by cyclization of thiosemicarbazide resin. The thiosemicarbazide resin is produced by the addition of various benzhydrazides to the isothiocyanate-terminated resin and serves as a key intermediate for the linker resin. This core skeleton 2-amino-1,3,4-oxadiazole resin and 1,3,4-thiadiazole resin undergoes functionalization reaction with various electrophiles such as alkyl halide and acid chloride to generate N-alkylamino and N-acylamino-1,3,4-oxadiazole and 1,3,4-thiadiazole resin respectively. Finally, 2-amino and 2-amido-1,3,4-oxadiazole and 1,3,4-thiadiazole derivatives are then generated in good yields and high purities by cleavage of the respective resin under trifluoroacetic acid(TFA) in dichloromethane(DCM).

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Design and Synthesis of Unprecedented Thienopyrazine Derivatives as a Trasnglutaminase 2 inhibitor

김나연 JUVEKARVINAYAK 공영대*

동국대학교 화학과

Overactivity of trasnglutaminase 2 (TGase 2) influences inflammation and cancer. We have identified the anticancer effect of GK-13, 2-(phenylethynyl)-3-(2-(pyrrolidin-1-yl)ethoxy)quinoxaline, which is associated with its inhibition against TGase 2. In the optimization process, we developed a novel core skeleton of thieno[3,4-*b*]pyrazine through the modification of GK-13 which was a lead compound in previous studies. Some of the thieno[3,4-*b*]pyrazine derivatives were shown to hold promise for use as potential therapeutic small-molecules in cancer treatment through the inhibition of the activity of TGase 2. Especially, compared to GK-13, GK-428, N,N-dimethyl-3-((3-(phenylethynyl)thieno[3,4-*b*]pyrazin-2-yl)oxy)propan-1-amine, showed a higher prospect as an TGase 2 inhibitor. Furthermore, we carried out the docking study of both GK-428 and GK-13 to provide a rationale explanation for the active sites of the Transglutaminase 2 structure.

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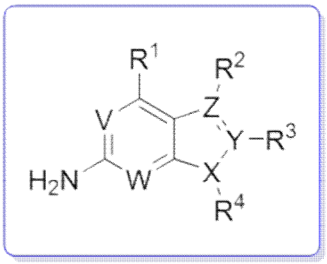
Novel 2-Aminopurine Derivatives as Hsp90 Inhibitors; Synthesis, X-ray Crystallographic Studies and Biological Evaluation for Anticancer agents

이주현 신상철[1] 서선희[2] 강순방[2] 정낙철 금교창[3,*]

고려대학교 화학과 [1]한국과학기술연구원(KIST) 의공학연구소 테라그노시스연구단 [2]한국과학기술연구원(KIST) 뇌의약연구단 [3]한국과학기술연구원(KIST) 케모인포메틱스연구센터

Heat-shock protein 90 (Hsp90), an ATPase-dependent protein folding molecular chaperone, regulates the stability and function of many client proteins such as Src, cdk4, Akt, HER2/neu, EGFR, c-Kit, and Raf-1. Many of misfolded client proteins play critical roles in cancer progression. Hence, inhibition of Hsp90 leads to destabilize the client proteins by conformational change of between Hsp90 and client proteins. And then, these oncogenic client proteins undergo degradation via ubiquitin-dependent pathway. Development of Hsp90 inhibitors has been extensively studied as a target of cancer therapy. Among Hsp90 inhibitors, we are interested in the purine based inhibitors such as CUDC-305, PU-H71, MPC-3100, and BIIB021.Herein, a series of 2-aminopurine derivatives were synthesized, and evaluated against SKBR3, MCF-7, and HCT116 cancer cell lines. Several compounds displayed good anti-proliferative activities in in vitro assay, and also showed high binding affinity for N-terminal Hsp90α in ITC and FP competition assay. Among them, KKK5142 showed highest binding affinity similar to BIIB021 in FP competition assay. Moreover, X-ray crystallographic data of KKK5142-Hsp90 complex demonstrated that KKK5142 bound in the N-terminal ATP-binding domain with stable binding conformation. The ring substituents at N-7 position displayed hydrophobic interaction with Leu107, and aryl ring at N-9 position exhibited π-π stacking interaction with Phe138 in the hydrophobic pocket by reserving the conformation of outer helix.


R1
R2
Z
V
Y
R3
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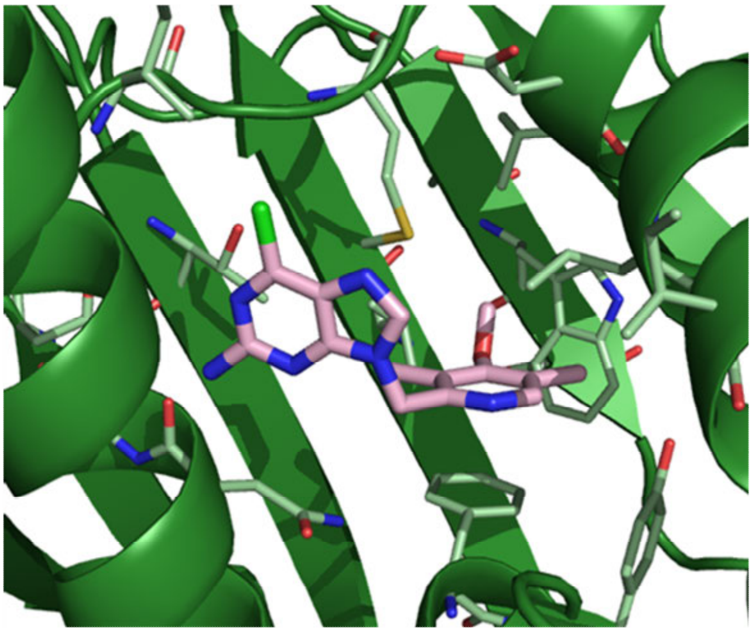
X
R4



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발표분야: Oral Presentation for Young Medicinal Chemists
발표종류: 구두발표, 발표일시: 금 11:00, 좌장: 윤창수

Development of Small Molecules and Chemical Probes as Potential HIF (Hypoxia Induced Factor)-1α Inhibitors

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동국대학교 약학과 [1]동국대학교 약학대학

Interest in the role of hypoxia-inducible factor 1 (HIF-1) in cancer biology has grown exponentially in the two decades since its identification. Hypoxia inducible factor (HIF) 1 is a key transcription factor that functions as a mast regulator in the response of growing tumor to hypoxia. Tumor hypoxia has been recognized as a common feature of solid tumor and a negative prognostic factor for response to treatment and survival of cancer patients. HIF-1α plays a major role in activating gene transcription and is important for maintaining homeostasis under hypoxic conditions. HIF-1α is a potential target for the development of novel cancer therapeutics. In an attempt to develop a novel small molecule inhibitor targeting HIF-1α protein in solid tumor, we conducted phenotype-based structure activity relationship (SAR) study along with chemical biology techniques using multifunctional chemical probes. Photoaffinity labeling, click conjugation, and biotinylation, are very useful tools for detecting target proteins of biologically active molecules. On the basis of this approach, we designed and synthesized series of small molecules as well as multifunctional chemical probes and evaluated as HIF-1α inhibitors. Some of the compound showed good to excellent activity against HIF-1α, which suppressed hypoxia-induced HIF-1α accumulation and target gene expression in a dose-dependent manner. Further results from medicinal chemistry and target identification work will be discussed.

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발표코드: **MEDI.O-6**
발표분야: Oral Presentation for Young Medicinal Chemists
발표종류: 구두발표, 발표일시: 금 11:15, 좌장: 윤창수

Target Identification Revealed the Direct HMGB2-binding Small Molecule with Anti-neuroinflammatory Effect

이상희 박승범[*]

서울대학교 화학부

Neuroinflammation, mainly considered as multiple immune responses in central nervous system, is highly associated with activation of microglia. Microglia-mediated neurotoxicity results in neuronal damage and death, which eventually attributes to neurodegenerative diseases. Due to the crucial role of neuroinflammation in brain diseases, there is a significant unmet need for the identification of potential therapeutic target as well as the discovery of their novel therapeutic agents towards neurological diseases. In this presentation, discovery of a novel anti-neuroinflammatory agent, Inflachromene (ICM), and the identification of its molecular target using FITGE (Fluorescence difference In Two-dimensional Gel Electrophoresis) technology are discussed. Based on the integration between phenotypic screening and subsequent target deconvolution, we successfully identified direct binding target of ICM as high mobility group box 2 (HMGB2) for preventing neuroinflammation and suggested a great therapeutic effect on *in vitro* and *in vivo* system. Particularly, ICM is the first HMGB2 binding-small molecule. The fact that ICM delicately modulates the activity of multifunctional HMGB by perturbing the post-translational modification of HMGB2 demonstrates the value of ICM as a research tool for HMGB study.

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발표분야: Oral Presentation for Young Medicinal Chemists
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Apoptosis imaging studies in various animal models using radio-iodinated peptide

하영수 Nisarg R. Soni 이웅희 안광일[1] 유정수[*]

경북대학교 의과대학 분자의학교실 [1]한국원자력의학원 방사성의약품 개발실

Apoptosis has a role in many medical disorders and treatments; hence, non-invasive evaluation of programmed cell death is currently one of the most riveting research topics. Annexin V is the most widely used protein for apoptosis imaging. However, many problems, including high background, slow body clearance, and a need for calcium binding to phosphatidylserine, make it a suboptimum marker for apoptosis imaging. In this study, we radiolabeled the recently identified histone H1 targeting peptide ApoPep-1 and evaluated its potential as a new apoptosis imaging agent in various animal models.Results: The peptide was radiolabeled at high purity, and it showed reasonably good stability in serum for up to 5 hours. Cell death was easily imaged by radiolabeled ApoPep-1 in an ischemia surgery model, and liver apoptosis was more clearly identified by ApoPep-1 than [^{124}I]annexin V in cycloheximide-treated models. Three doxorubicin doses inhibited tumor growth by inducing apoptosis, which was confirmed by 30-40% decreases of [^{18}F]FDG and [^{18}F]FLT PET uptake in the tumor area. ApoPep-1 demonstrated more than 200% increase in tumor uptake after chemotherapy, while annexin V did not demonstrate any meaningful uptake in the tumor compared with the background. Biodistribution data were also in good agreement with the microPET imaging results.Conclusion: All of the experimental data clearly demonstrated that apoptosis could be clearly imaged by radiolabeled ApoPep-1 peptide. [^{124}I]ApoPep-1 demonstrated better efficiency and versatility in various apoptosis detection than [^{124}I]annexin V.

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장소: 일산KINTEX

발표코드: **MAT.O-1**

발표분야: Current Trends in Materials Chemistry

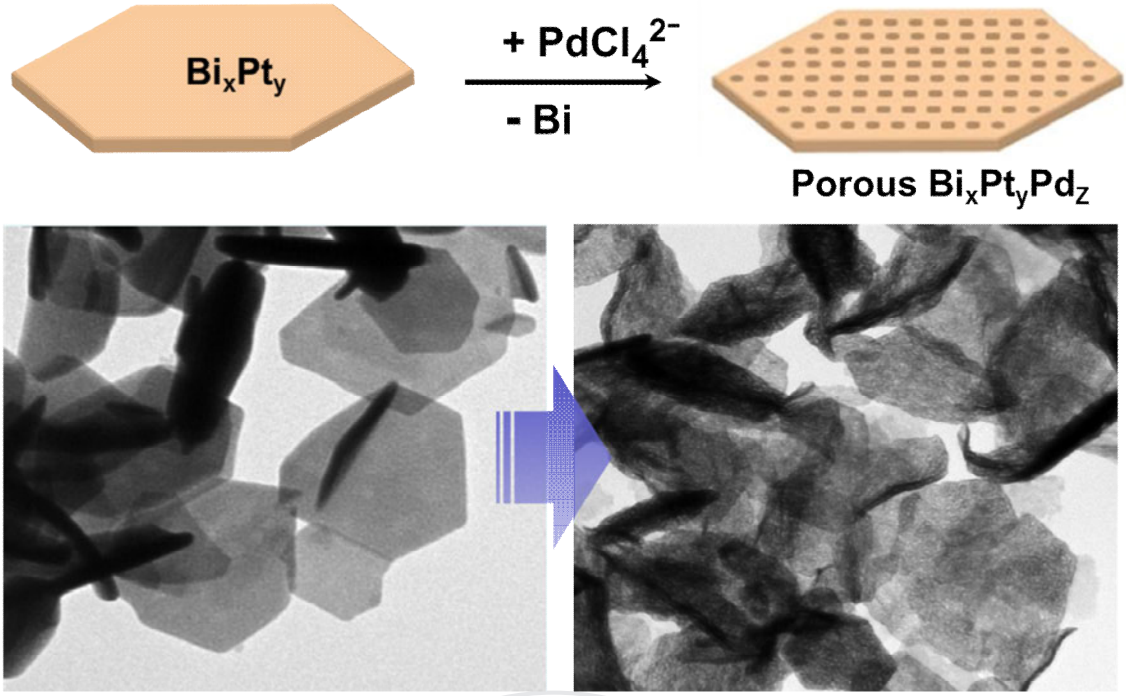
발표종류: 구두발표, 발표일시: 금 10:00, 좌장: 노준홍

Fabrication of $Bi_xPt_yPd_z$ alloy nanoporous plates with electro-catalytic activity

이강열

고려대학교 기계공학부

We demonstrate the fabrication of $Bi_{21}Pt_{35}Pd_{44}$ alloy porous nanoplates by a galvanic replacement method using Bi65Pt35 bimetallic nanoplates as the sacrificial template. $Bi_{65}Pt_{35}$ nanoplates, prepared by reduction with diol (1,2-hexadecanediol) at low temperature (100 °C), were converted to the porous nanoplate structure by a K_2PdCl_4/water/ethanol (1/1, v/v) mixed solution via galvanic replacement between bismuth and palladium. The formation of $Bi_{21}Pt_{35}Pd_{44}$ porous nanoplates is attributed to disperse crystallization under conditions of high nucleation rate. The electro-chemically active surface area (ECSA) for the $Bi_{21}Pt_{35}Pd_{44}$ alloy porous nanoplate is measured to be 0.943 cm^2. This value is 3 times greater than the ECSA (0.283 cm^2) of the commercial Pt/C (Alpha, Pt 20%) electrode. The electro-catalytic activity of the prepared porous nanoplates was examined for the oxidation of methanol in acidic solution. The $Bi_{21}Pt_{35}Pd_{44}$ porous nanoplates can effectively catalyze oxidation of methanol in acidic solution, probably owing to their larger surface area and many active reaction sites. The $Bi_{21}Pt_{35}Pd_{44}$porous nanoplates provide a new form of unsupported catalysts in contrast to the traditional supported nanoparticle catalyst and can be uniformly synthesized and separated easily from the reaction mixtures without aggregation.


Bi_xPt_y
$+ PdCl_4^{2-}$
$- Bi$
Porous $Bi_xPt_yPd_z$

일시: 2014년 4월 16~18일(수~금) 3일간
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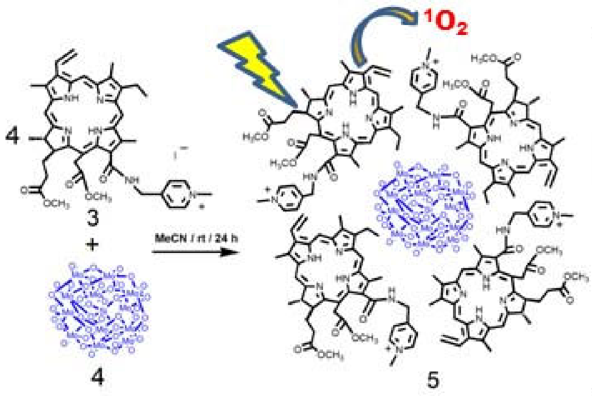
발표코드: **MAT.O-2**
발표분야: Current Trends in Materials Chemistry
발표종류: 구두발표, 발표일시: 금 10:20, 좌장: 노준홍

Efficient Photosensitization by a Chlorin?Polyoxometalate (POM) Supramolecular Complex

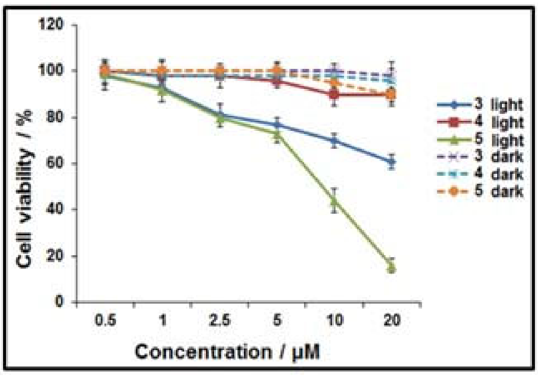
윤일* 심영기[1,*]

인제대학교 PDT 연구소 [1]인제대학교 나노공학부

Photodynamic therapy (PDT) is a promising noninvasive cancer treatment based on the activation of a photosensitizer (PS) upon light irradiation for the generation of reactive oxygen species to destroy thetumors. The development of desirable PSs as well as delivery systems of PSs has attracted much attention for highly selective targeting of tumor sites. Cationic chlorins or porphyrins have advantages compared to neutral (nonionic) chlorins or porphyrins for higher uptake and retention for tumor targeting,which has potential applications such as DNA binding and photocleavage and PSs for PDT.Polyoxometalates (POMs), well-defined early-transitionmetaloxygen anion clusters, have attracted extensive interest because of their intriguing properties including catalytic, electronic, optical, and magnetic functionalities. In addition,POMs have interesting medicinal properties such as antitumor and antiviral activities. However, there are very rare reports for medicinal applications usingPOM and organic molecules. This is the first example of an inorganic?organic hybrid molecular assembly using POM and chlorin (the PS) molecules that can enhance the photodynamic activity against the cell lines. The 4:1 supramolecular complexed ionic salt between pyridinium chlorin and polyanionic [α-SiMo12O40]4? exhibits significantly enhanced photodynamic activity against A549 cell lines because of increased singlet oxygen photogeneration through high cellular penetration and localization of the chlorin molecules on the ionic salt into the cancer cell. Confocal laser scanning microscopy images clearly represent a higher uptake and photodynamic effect of this supramolecular complex corresponding to the lower IC50 value compared to the free chlorin.



4
3
+
4
5
MeCN / rt / 24 h
$^1O_2$
I^-



Cell viability / %
120
100
80
60
40
20
0
0.5
1
2.5
5
10
20
Concentration / μM
3 light
4 light
5 light
3 dark
4 dark
5 dark

일시: 2014년 4월 16~18일(수~금) 3일간
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발표분야: Current Trends in Materials Chemistry
발표종류: 구두발표, 발표일시: 금 10:40, 좌장: 노준홍

Mussel-Inspired Polydopamine Films for Biopolymer-Based Optoelectronic Devices

남혜진 정덕영[1,*]

성균관대학교 기초과학연구소 [1]성균관대학교 화학과

New polydopamine (PDA)-based optoelectronic devices including dye-sensitized solar cells (DSSCs) and organic phototransistors (OPTs) were first demonstrated. Spontaneously self-polymerized PDA using dip-coating (DC) and cyclic voltammetry (CV) were applied to TiO_2 layers under a nitrogen atmosphere as a photosensitizer for DSSCs. Both synthetic methods led to excellent photovoltaic results by direct dye-to-TiO_2 charge transfer and the PDA-DC exhibited larger current density and cell efficiency values than those for the PDA-CV. The PDA showed strong adhesion to the nanocrystalline TiO_2 electrodes and the interface were studied through the control of the coating methods, reaction times and solution concentration in order to maximize the conversion efficiency. On the other hand, PDA thin film with a dense and conformal surface was prepared by self-polymerization using O_2 gas as an oxygen source instead of a conventional air stream. The PDA exhibited ultra-high photoresponsivity and efficient light detection ability in OPTs. The single-step deposition process and precise control of the PDA thin film by micropatterning led to fabricate high-performance OPTs. The excellent device performance producing an extremely high photocurrent at a low voltage provides potential applications in low-cost, high-density organic optoelectronics.

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발표분야: Current Trends in Materials Chemistry
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TiO2 Nanotubes Fabrication with Tunable Exposed (001) Facets for Enhanced Conversion Efficiency of Solar Cells

정미희

한국전자통신연구원 박막태양광기술연구팀

We have demonstrated that the use of poly(vinyl pyrrolidone) (PVP) and acetic acid during the synthesis of TiO2 nanotubes (NTs) may result in a synthesis of anatase TiO2 nanocrystals with exposed, chemically active (001) facet. In the present experiment, PVP in the electrolyte solution acts as a surfactant and controller of crystal growth. PVP were preferentially adsorbed onto the (101) surfaces, so the growth of (001) facets proceeded more quickly and prepared a single crystalline anatase exposing mainly the (001) plane. An enhancement in dye-sensitized solar cells (DSSCs) overall conversion efficiency is observed for the photoanode consisting of TiO2 single crystalline anatase exposed (001) facets. Experimentally confirmed by dark current potential and open circuit voltage decay scans, such highly exposed (001) facets are not only favorable for more dye adsorption but also effectively retard the charge recombination process in DSSCs.

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Enhanced cellulose degradation by nano-complexed enzymes

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전남대학교 바이오에너지공학과

Current approaches for the conversion of lignocellulosic biomass to ethanol involve enzymes to complete the process of converting polysaccharides into fermentable sugars. As possible industrial catalysts for biomass conversion, enzymes have the potential to provide high specificity, low energy or chemical consumption, or low environment pollution. However, the high cost of enzymes is a key barrier to economic production of lignocellulosic ethanol. One promising strategy for reducing costs is the immobilization of enzymes in or on solid materials, which can potentially improve stability, storage properties, and enzyme reusability. This research describes the hydrolytic degradation of cellulosic biomass using cellulases(endo-glucanase, exo-glucanase, and β-glucosidase) and nano-complexed enzymes. Nano-complexed enzymes were prepared by immobilizing three kinds of cellulases onto nano particles (gold nanoparticles & gold-doped magnetic silica nanoparticles). The biochemical properties, stabilities, and hydrolytic activities of nano-complexed enzymes were compared to free cellulases. Furthermore, we observed the reusability of nano-complexed enzymes.

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Citric acid-assisted semi-wet combustion synthesis and characterization of nano-sized $LiFe_{0.95}Ti_{0.05}PO_4$ and $LiFePO_4$ cathode materials for Li-ion batteries

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울산대학교 화학과

A novel, cost effective, environment-friendly and energetically beneficial alternative method for the synthesis of nano-sized $LiFePO_4$ and $LiFe_{0.95}Ti_{0.05}PO_4$, $Li_{2.5}Fe_{0.9}5Ti_{0.05}PO_4$ and $LiFe_{0.95}Ti_{0.05}PO_4/C$ cathode material by sol-gel and semi-wet combustion synthesis is presented. The method involved auto-combustion of an aqueous precursor solution in oxygen atmosphere with the help of external fuels and is capable of producing high amount of $LiFePO_4$ and $LiFe_{0.95}Ti_{0.05}$ PO_4 at ultra-low temperature in the combustion residue itself. The amount of phase generated was observed to be highly dependent on the combustion process i.e. on the nature and amount of external-fuels added for combustion. On a structural characterization grain size was observed to decrease drastically to nano-dimension compared to submicron-size that was obtained in a traditional sol-gel combustion and subsequent calcination method. Therefore, the method reported can produce nano-crystalline $LiFePO_4$ and $LiFe_{0.95}Ti_{0.05}PO_4$ at an ultra-low temperature and is expected to be applicable for cathode materials. The crystal structure and electrochemical behavior of the materials were investigated using TG/DTA, X-ray diffraction, SEM, EDX, TEM, XPS, cyclic voltammetry, and charge/discharge cycle measurements. It was found that the electrochemical behavior of $LiFePO_4$ could be increased by Ti-doping method.

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Solid-State Asymmetric Supercapacitor based on Manganese Dioxide/Reduced-Graphene Oxide and Polypyrrole/Reduced-Graphene Oxide in a Gel Electrolyte

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Manganese dioxide/reduced graphene oxide/indium tin oxide (MRI) and polypyrrole/reduced graphene oxide/indium tin oxide (PRI) electrodes were prepared via the chronopotentiometric- deposition of either manganese oxide or polypyrrole, respectively, onto a RGO/ITO film at a constant current density. Solid-state asymmetric supercapacitors (ASC) were assembled using MRI as the positive electrode and PRI as the negative electrode in a PVA/LiCl gel electrolyte. These devices displayed a power density of 7.4 kW/kg (for an energy density of 13 Wh/kg), an energy density of 16 Wh/Kg (for a power density of 0.3 kW/kg), and a capacitance retention of 75% over 2000 cycles. The MRI//PRI ASC exhibited a much improved capacitive performance compared to the symmetric PRI//PRI (3 Wh/kg at 0.47 kW/kg) and MRI//MRI (9 Wh/kg at 0.12 kW/kg) supercapacitors. The superior capacitive performance of the MRI//PRI ASC was ascribed the improved conductivities and mechanical stabilities of MRI and PRI electrodes, obtained by preparing the polypyrrole and manganese oxide films on a graphene-coated electrode.

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Ultrathin Multilayer Poly(*p*-phenylene vinylene)/Reduced Graphene Oxide: Film as an Efficient Organic Current Collector in a Flexible Carbon-based Supercapacitor

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We describe the preparation of an all-solid-state flexible in-plane supercapacitor based on a poly(ethylene terephthalate) (PET) substrate, laminated with two strata of ultrathin multilayer films composed of 30 polyaniline (PANi)/reduced graphene oxide (RGO) bilayers, and 30 poly(*p*-phenylene vinylene) (PPV)/RGO bilayers. The influence of the $(PPV/RGO)_{30}$ stratum on the electrochemical properties of the $(PANi/RGO)_{30}/(PPV/RGO)_{30}$ film (denoted P30) supported on a PET was evaluated and compared with the corresponding influence of the (PANi/RGO)53 film (denoted P53). The P30 and P53 films were prepared with similar thicknesses (90.1 and 91.5 nm, respectively). The volumetric capacitance of P30 at a discharge current of 20 A/cm^3 (957 F/cm^3) was much higher than that obtained from P53 (733 F/cm^3), indicating that the $(PPV/RGO)_{30}$ film performed well as a current collector. The electron transfer resistance of the P30 electrode was found to be nearly 59% of the corresponding value of P53 (1.53 kΩ cm^2 vs. 2.60 kΩ cm^2, respectively). Furthermore, an all-solid-state flexible in-plane EC assembled with P30 electrodes in the parallel mode (denoted EC30) exhibited an outstanding volumetric capacitance (152 F/cm^3 at 20 A/cm^3) with a high energy density (9.4 mWh/cm^3) and power density (6.5 W/cm^3). EC30 performed well under long-term cycling tests, retaining 85% of its initial capacitance retention after 1000 charge/discharge cycles. The excellent electrochemical properties of EC30 may potentially meet the requirements for miniaturized electrodes in the manufacture of flexible, lightweight, mechanically durable microelectronic applications.

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Strongly-Coupled 2D Nanohybrids of Titanate?Graphene with Novel Functions as Photocatalysts and Antibacterial Matrices

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Strongly-coupled two-dimensional (2D) nanohybrids of titanate-reduced graphene oxide (rG-O) nanosheets are synthesized in the form of powdery composite and freestanding film. A reassembling reaction between TiO2 nanoparticles and rG-O nanosheets yields the powdery nanohybrid of layered titanate-rG-O through a phase transformation of anatase TiO2 to layered titanate. The hybridization with rG-O nanosheets is effective not only in promoting the phase transition of anatase TiO2 to layered titanate but also in improving the thermal stability of layered titanate, indicating the role of rG-O nanosheet as an agent for directing and stabilizing layered structure. Of prime interest is that the hybridization with rG-O nanosheets suppresses an absorption edge of semiconducting titanate component, strongly suggesting a modification of the electronic structure of titanate component upon the hybridization with rG-O. A strong electronic coupling between two components is evidenced by the visible light-induced generation of photocurrents after the hybridization with rG-O. Another form of titanate-rG-O freestanding film can be fabricated by a vacuum-assisted filtration of the mixed colloidal suspension of titanate and rG-O nanosheets. The stability of the freestanding film for the microwave and ultrasonic stresses becomes remarkably enhanced upon the incorporation of layered titanate nanosheets, a result of strong coupling between interstratified rG-O and layered titanate nanosheets. Also, the incorporation of layered titanate nanosheets into the rG-O paper remarkably enhances the antibacterial properties and hydrophilicity of the graphene paper, which is attributable to the increase of surface roughness. The present findings clearly demonstrate that the hybridization of 2D titanate and rG-O nanosheets is fairly powerful in optimizing the photocatalytic and antibacterial functionalities of metal oxide-based nanohybrids.

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중등 예비과학교사의 교육과정 설계에서 교육과정 자료의 활용 방식 분석

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이 연구에서는 사례연구를 통해 중등 예비과학교사의 교육과정 설계에서 교육과정 자료의 활용 방식을 조사하였다. 서울 소재 사범대학에 재학 중인 두 명의 예비과학교사가 연구에 참여하였다. 교수학습관에 대한 사전면담을 실시한 후, 교육실습 기간 동안 이루어진 각 예비교사의 수업을 관찰하였고, 모든 교수학습 자료를 수집하였으며, 수업 실행 전후에 반구조화된 면담을 진행하였다. 예비교사들의 교육과정 자료의 활용 방식을 읽기, 평가, 응용의 측면에서 체계적으로 분석한 결과, 두 예비교사의 교육과정 설계에서 교육과정 자료의 활용 방식에 상당한 차이가 있었다. 교육과정 자료에 대한 읽기의 방식에 차이가 있었는데, 이는 두 예비교사의 교육과정 재구성에 대한 관점의 차이로부터 비롯되었다. 교육과정 재구성에 대한 관점의 차이는 교육과정 자료의 응용 방식에도 영향을 미쳐서 교육과정 재구성에 대해 적극적인 관점을 지닌 경우 '구성요소 추가'가, 소극적인 관점을 지닌 경우 '구성요소 변형'이 중요한 응용 방식이었다. 또한, 예비교사의 교수학습관에 따라 교육과정 자료를 평가하는 과정에서 학습자를 고려하는 수준에 차이가 있었다. 평가에서의 이러한 차이는 '교사중심활동의 증가'와 '학생중심활동의 증가' 응용에서의 질적인 차이로 연결되었다. 이에 대한 교육적 함의를 논의하였다.

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중학교 과학, 고등학교 화학 ⅠⅡ 교과서에서 제시된 실험의 안전에 관한 내용 분석

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2009 개정 교육과정에서 과학교과서에서는 탐구활동 중심의 학습이 이루어지도록 강조하고 있다. 실험은 과학교과의 가장 기본적인 활동이자 동시에 안전사고의 위험이 항상 수반된다. 학생과 교사가 가장 기본적으로 사용하는 교과서에 각 실험활동을 수행하기 전에 숙지해야 할 실험 안전에 관한 내용이 많이 부족하다는 것을 선행연구를 통해 인지하였다. 교과서에 제시된 실험마다 실험 안전에 대한 내용이 충분히 반영되었는지에 대한 연구의 필요성을 바탕으로 본 연구에서는 2013 년도에 발행된 교과서를 기준으로 과학 및 화학수업에서 요구되는 실험들 중에 특별히 안전에 유의해야 하는 실험들을 중심으로 일반적인 안전수칙안내를 제외한 중학교 과학 교과서(1 학년 9 종, 2 학년 6 종, 3 학년 5 종)와 화학 Ⅰ(4 종) 및 화학 Ⅱ(4 종)을 모아서 서울시교육청에서 배포한 중고등학교 과학 실험실 안전지도서에서 제시된 주의해야할 실험 중 중학교 교과서내 5 가지실험과 고등학교 교과서내 8 가지 실험을 각 교과서에서 제시된 실험도구 및 실험방법과 실험에서 안전상의 유의점 내용을 비교 분석하였다. 본 연구를 토대로 실험 안전에 대한 중요성을 교사와 학생 모두에게 고취시키고 좀 더 체계적이고 실질적인 실험 안전 내용을 교과서에 수록 할 수 있는 기초자료를 제공하고자 한다.

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2009 과학과 교육과정의 선택과목 편성 및 현황 조사

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이 연구의 목적은 2009 개정 교육과정에 따라, 고등학교에서 과학과 교육과정의 일반 과목이 어떻게 선택되어 편성되고 있는가를 조사하고 분석하는 것이다. 이를 위하여, 전국 17 개 시도교육청의 일반계 고등학교 418 개교를 대상으로, 한국과학창의재단 및 시·도 교육청의 협조를 얻어 교육과정 편성운영 현황을 조사하였다. 그에 대한 연구결과는 다음과 같다, 첫째, 2011 년에서 2013 년까지 연도가 올라갈수록, 과학을 선택하는 학생 수가 줄어드는 반면, I 과목의 선택 학생수가 늘어나는 것으로 조사되었다. 둘째,선택과목 I 의 경우, 생물, 지구과학, 화학, 물리의 순서로 학생들이 많이 선택하는 것으로 조사되었다. 화학과 물리를 선택하는 학생의 각각 비율은 생물의 2/3 수준에 해당하는 것으로 나타났다. 셋째, 선택 과목 II 의 경우, 연도가 올라갈수록 모든 선택과목에 있어서 학생들이 선택하는 비율이 점차 줄어드는 경향이 나타났다. 넷째, 인문사회계 학생들이 인문사회계열 과목과 자연계열 과목을 배우는 것과, 자연계열 학생들이 자연계열 과목과 인문사회계열 과목을 배우는 것을 비교할때, 자연계열 학생들이 자연계열 과목을 배우는 비율이 인문사회계열 학생들이 인문사회계열 과목을 배우는 비율보다 적은 것으로 조사되었다. 또한 자연계열 학생들이 인문사회계열 과목을 배우는 비율은 인문사회계열 학생들이 자연계열 과목을 배우는 비율보다 많은 것으로 나타났다. 이러한 결과를 통해 중등학교에서의 화학 교과의 문제점에 대한 인식을 하고, 과학자, 과학교육자, 교육자 등 관련자들이 총체적으로 그 해결책에 대하여 논의하는 계기가 되길 기대하는 바이다.

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학교현장실습 기간 중 e-멘토링 운영에 대한 예비교사와 실습 지도교수의 인식

차정호* **오정숙**[1] **백상수**[2]

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이 연구에서는 학교현장실습(구 교육실습) 기간 중 e-멘토링의 운영 전반에 대한 중등 예비교사와 실습지도교수의 인식을 조사하였다. 경북 지역에 위치한 사범대학의 4학년 학생 134명(남 33명, 여 101명)과 실습 지도교수 23명(남 13명, 여 10명)을 대상으로 설문을 실시하였다. 분석결과, 예비교사들은 e-멘토링을 통해 교육활동 계획, 실시, 평가에 대해 지도받기를 희망하였고, 지도교수에게는 정기적이고 규칙적인 피드백을 제공하는 역할에 대한 기대가 가장 컸다. 또한 예비교사의 역할에 대해 실습지도교수와 동료들로부터 적극적으로 배워야한다고 인식하였고, 바람직한 교수와 학생 비율에 대해서는 교수 1명과 실습생 2-3명을 선호하였다. 실습 지도교수들의 경우, e-멘토링 활동을 통해 예비교사들의 교육활동 계획, 실시, 평가를 지도해야 한다고 생각하였고, 실습생의 어려움을 듣고 나누고자 하는 인식도 높았다. 멘토의 역할로서 실습생이 직면한 문제를 스스로 해결하도록 지원하는 것을 가장 중요하게 인식하였다. 또한 예비교사의 역할에 대해서는 실습 지도교수 및 동료들과 정보를 교류하고 공유하는 것을 중요하게 생각하였다. 멘토링 그룹의 교수와 학생 비율에 대해서는 교수 1명과 실습생 4-5명이 가장 적절하다고 응답하였다. 연구결과를 바탕으로 추후 연구에 대한 시사점과 후속 연구를 제안하였다.

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초등과학 디지털교과서를 활용한 수업의 특징 분석

오현민 임희준*

경인교육대학교 과학교육과

디지털기술의 빠른 발달은 현대사회 전반의 변화를 이끌고 있으며 교육분야에도 디지털기술의 도입은 점진적으로 이루어지고 있다. 특히 디지털교과서의 도입은 기존 교과내용에 용어 사전, 멀티미디어 자료, 평가문항, 보충·심화학습 내용 등 풍부한 학습자료와 학습지원 및 관리기능이 부가되어 학습자의 학습효율을 높여줄 것으로 기대되어지고 있다. 본 연구는 디지털교과서를 활용한 교수학습에서의 수업의 흐름과 상호작용을 분석하였다. 첫째, 디지털교과서는 수업 시간에 교과서 내용 보기, 동영상 및 사진 보기, 실험관찰 기록하기, 평가 등에만 국한되어 사용되고 있었다. 둘째, 디지털교과서를 통한 특별한 상호작용은 나타나지 않았다. 셋째, 디지털교과서를 사용한다고 해서 일반적인 교수학습의 흐름과 달리 특별한 수업 방법은 나타나지 않았다. 이러한 결과를 토대로 볼 때, 디지털교과서를 효과적으로 활용할 수 있도록 하는 콘텐츠의 개발과 교수학습 전략의 개발의 필요함을 알 수 있다.

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발표분야: Recent Trends in Chemistry Education

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문제 유형에 따른 초등 영재 학생들의 문제해결과정 연구

임희준

경인교육대학교 과학교육과

본 연구는 초등학교 6 학년 영재학급 학생 중 6 명을 대상으로 문제 유형에 따른 초등 과학영재 학생의 문제해결과정에 대한 특징을 분석하였다. 문제해결과정을 알아보기 위한 과학 문제로는 논리성을 요구하는 문항, 개방성을 요구하는 문항, 논리성과 개방성을 동시에 요구하는 문항 각 2 문항씩 총 6 문항을 사용하였다. 사례 연구를 통한 질적 분석을 하기 위해 발성 사고법을 이용해 면담 자료를 수집하였으며 수집된 자료는 전사 자료를 바탕으로 한 문제해결과정 분석틀을 이용해 문제해결과정별 유형에 따른 특징을 분석하였다. 그리고 문제이해-계획수립-계획실행-검토반성의 문제해결과정의 하위요소에서 나타나는 특징을 살펴보았다.

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중학교 과학 학습 부진학생의 원인 유형별 프로그램 개발 및 적용

이경희 최병순*

한국교원대학교 화학교육과

이 연구의 목적은 과학학습부진을 해소하기 위해 과학학습부진 원인에 따라 맞춤형 지도를 할 수 있는 프로그램을 개발하고 적용하여 그 효과를 보는 것이다. 이를 위해 과학학습부진 특성 및 원인을 분석하여 주요 원인을 중심으로 과학탐구능력 부족형, 과학학습동기 부족형, 과학학습전략 부족형 등 3 가지 유형으로 구분하였고, 원인 유형별 프로그램을 개발하였다. 이 프로그램은 방과후 학교 프로그램으로 2009 개정 교육과정 7 학년 과학교과 내용을 이해하기 쉽게 재미있는 활동 중심으로 구성하였고, 3 가지 원인인 탐구능력, 학습동기, 학습전략능력이 향상될 수 있는 요소들을 포함하였다. 프로그램의 효과를 보기 위해 충청북도 청주시에 소재한 M 중학교 1 학년 과학학습부진아 22 명 중 원인 유형 검사를 통해 비교집단 11 명, 실험집단 11 명(3 유형으로 구분)을 선정하였으며, 동일 단원과 주제로 비교집단은 기본 개념과 활동 중심의 수업을 실시하고 실험집단은 원인 유형별 프로그램을 주 1 회, 60 분씩 18 주 동안 실시하였다. 프로그램에 대한 인식검사, 과학탐구능력 검사, 학습동기 및 학습전략 검사, 학업성취도 평가를 하였으며, 학생활동지, 연구일지, 수업내용전사, 학생면담 등을 통해 프로그램 효과를 보았다. 연구 결과, 실험집단에서 과학학습부진 원인 유형별 프로그램에 대해 높은 만족도를 보였고, 과학에 대한 흥미와 학습의욕이 생겼으며, 과학개념에 대한 이해가 용이하였다고 응답하였다. 또한, 3 가지 부진 유형에서 탐구능력, 학습동기, 학습전략능력이 각각 향상되었고, 더불어 학업성취도도 향상되었다. 수업 과정에서 나타난 학습 태도 면에서도 전반적으로 적극적이고 긍정적인 태도로 변하였다. 과학학습동기 부족형과 과학학습전략 부족형의 학생들은 다른 원인까지도 더불어 향상되는 경향을 보였다. 이는 학습동기나 학습전략은 정의적인 영역으로 부진 원인이 점차적으로 해소되어 나가면서 학생 스스로 과학학습에 대한 관심과 흥미를 가지게 되고, 수업에 임하는 과학학습 태도가 긍정적으로 변해가면서 다른 부진 원인 요인에도

긍정적인 영향을 미친 것으로 여겨진다. 이러한 결과는 과학학습부진 원인 유형별 프로그램이 과학학습부진아들을 지도하는 데 유용한 자료로 활용될 수 있음을 보여준다.

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새로운 교육 동향, 사회정서학습(Social Emotional Learning, SEL)과 과학교육

박현주

조선대학교 과학교육학부

사회정서학습(Social Emotional Learning, SEL)은 지금까지 교육현장에서 당연하다고 여겨 외면하거나 무관심하였던 요소들을 교육의 장으로 끌어들여, 적극적으로 학생들의 인성교육에 포함하고자 하는 노력에서 비롯된다. 오늘날의 창의성과 가치는 긍정적인 자아와 집단 속의 협동과 경쟁과정을 거치면서 발휘되므로, 실제적인 과학교육과 SEL 을 연결하여 제시된 교육을 통하여 학생들의 인지적 성장과 정의적 성장이 유기적으로 이루어질 수 있도록 안내해야 한다. 이 연구는 SEL 의 개념과 발생을 살펴보고, 과학교육의 연결을 과학의 본성과 탐구의 관점에서 살펴보고자 한다. SEL 의 사회적(Social) 측면은 또래, 교사, 가족 등의 타인과의 긍정적 관계를 촉진하는데 초점을 두며, 개인간(interpersonal) 발달을 반영한다. 정서적(Emotional) 측면은 정서나 감정, 그리고 개인의 정서와 연결된 인지나 사고와 관련된 자기인식(self-awareness) 및 자기지식(self-knowledge)의 증진에 초점을 맞춘다. 학습(Learning) 측면은 사회적 및 정서적 영역에서의 성장과 적응이 수업, 연습, 피드백을 통해 가르치고 학습될 수 있다. SEL 은 지금까지 교육현장에서 당연하다고 여겨 외면하거나 무관심하였던 요소들을 교육의 장으로 끌어들여 적극적으로 학생들의 인성교육에 포함하고자 하는 노력에서 비롯된다. 오늘날의 창의성과 가치는 긍정적인 자아와 집단 속의 협동과 경쟁과정을 거치면서 발휘되므로, 실제적인 과학교육과 SEL 을 연결하여 제시된 교육을 통하여 학생들의 인지적 성장과 정의적 성장이 유기적으로 이루어질 수 있도록 안내해야 할 것이다.

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

Ethylene Polymerization with New Chromium Complexes Bearing [NNN]-heteroscorpionate Ligands

우정오 손경선*

충남대학교 화학과

We have developed a new family of chromium catalysts bearing [NNN]-heteroscorpionate ligands to explore the effects of the ligand structures on selectivity and productivity in ethylene oligomerization and polymerization. Here we present the synthesis and characterization of the new complexes as well as their catalytic behavior in ethylene polymerization.

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발표종류: 포스터, 발표일시: 수 16:00~19:00

A Tunable, Biocompatible, and Multifunctional Elastomers Based on Polyols

오성진 우정오 손경선*

충남대학교 화학과

We have developed a family of synthetic biodegradable elastomers composed of crosslinked networks based on polyols. Here we describe the synthesis and characterization of the new biocompatible elastomeric polymers to investigate their thermal/mechanical properties, degradation rates, and biocompatibility depending upon the crosslinking density and the type of polyols.

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발표코드: **POLY.P-3**

발표분야: 고분자화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis, Characterization, and Ethylene Oligomerization/Polymerization Studies of Chromium Complexes Containing Pyridyl and Pyrazolyl Ligands

박종은 손경선*

충남대학교 화학과

We have developed a new family of chromium complexes bearing pyridyl and pyrazolyl ligands, and the effects of ligand modification on the catalytic activity and selectivity were evaluated for ethylene oligomerization and polymerization. Here we present the polymerization results as well as the synthesis and characterization of the new Cr complexes

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발표코드: **POLY.P-4**

발표분야: 고분자화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Ring-opening Metathesis Polymerization of Norbornenes with Pendant PCBM for an Acceptor in OPVs: Comparison with Vinyl-type Polynorbornenes

김태원 김민지 이민형*

울산대학교 화학과

Polynorbornenes with pendant PCBM moieties (**RP1** and **RP2**) were produced by ring-opening metathesis polymerization (ROMP) of norbornene monomer functionalized with PCBM using a Grubbs second-generation catalyst. **RP1** possessed high decomposition temperature and moderate glass transition temperature, but was thermally cross-linked at 80 °C. While the bulk-heterojunction organic photovoltaic devices fabricated with the active layer comprising poly(3-hexylthiophene) (P3HT) donor and **RP1** acceptor at ambient temperature exhibited a power conversion efficiency of 0.66%, the efficiency decreased to 0.28% after pre-annealing of the active layer at 110 °C. In contrast, the devices based on the P3HT:vinyl-type polynorbornene bearing PCBM moiety (**P1**) active layer showed high thermal stability up to 150 °C with no decrease in the device performance. Details of synthesis and electron-accepting properties of polynorbornenes in OPVs will be discussed.

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발표종류: 포스터, 발표일시: 수 16:00~19:00

Morphological Control of Polymer Bulk Heterojunction Solar Cells Using Naphthodithiophene-Thienopyrrolodine based polymers

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포항공과대학교 화학공학과

The morphological control of polymer bulk heterojunction solar cells is demonstrated by tuning the surface energy of Naphthodithiophene-Thienopyrrolodine based polymers via end-groups modification, on which a photoactive layer composed of the nanoscale domain size of polymer:PCBM bulk heterojunction is formed. The BHJ morphology is examined using scanning electron microscopy and atomic force microscopy techniques. The microscopic results revealed that the clear correlation between the nanometer-sized morphology and well-matched surface energy of the donor/acceptor materials which leads to better donor/acceptor miscibility that promotes efficient exciton dissociation and bi-continuous percolating networks for charge collection efficiency and thus increase photovoltaic performance. These findings demonstrated that the surface energy control of the conjugated donor polymer is desirable for improving the efficiency of bulk heterojunction solar cells.

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

Efficient Stable Perovskite-Sensitized Solar Cells with Diketopyrrolopyrrole-Containing Hole Transporting Conjugated Polymer

강경호 임종철 박태호*

포항공과대학교 화학공학과

Alternative HTM materials with excellent electrical properties may be used in place of spiro-MeOTAD. Poly[2,5-bis(2-decyldodecyl)pyrrolo[3,4-c]pyrrole-1,4(2H,5H)-dione-(E)-1,2-di(2,2'-bithiophen-5-yl) ethene] (PDPPDBTE) was successfully incorporated as a p-type hole transporting material in solid-state organic?inorganic hybrid solar cells. The excellent optical and electrical properties of organo-lead halide perovskite (CH3NH3PbI3) nanocrystals used as a light harvester yielded a 9.2% power conversion efficiency (PCE) for the best-performing cell that exceeded the value (7.6%) obtained from the best hole conductor yet reported (2,2',7,7'-tetrakis(N,N-di-p-methoxyphenyl-amine)9,9'-spirobifluorene, spiro-MeOTAD). The high PCE was attributed to the optimal oxidation potential (5.4 eV) and excellent charge carrier mobility of the polymer. The hydrophobicity of the polymer prevented water permeation into the porous perovskite heterojunction, and long-term aging tests over 1000 hours confirmed the enhanced stability of the PDPPDBTE-based cells.

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Diketopyrrolopyrrole-Containing Hole Transporting Conjugated Polymer for use in Efficient Stable Organic-Inorganic Hybrid Solar Cells based on a Perovskite

임종철 김윤희[1] 박태호*

포항공과대학교 화학공학과 [1]경상대학교 화학과

Poly[2,5-bis(2-decyldodecyl)pyrrolo[3,4-c]pyrrole-1,4(2H,5H)-dione-(E)-1,2-di(2,2'-bithiophen-5-yl) ethene] (PDPPDBTE) was successfully incorporated as a p-type hole transporting material in solid-state organic?inorganic hybrid solar cells. The excellent optical and electrical properties of organo-lead halide perovskite ($CH_3NH_3PbI_3$) nanocrystals used as a light harvester yielded a 9.2% power conversion efficiency (PCE) for the best-performing cell that exceeded the value (7.6%) obtained from the best hole conductor yet reported (2,2',7,7'-tetrakis(N,N-di-p-methoxyphenyl-amine)9,9'-spirobifluorene, spiro-MeOTAD). The high PCE was attributed to the optimal oxidation potential (5.4 eV) and excellent charge carrier mobility of the polymer. The hydrophobicity of the polymer prevented water permeation into the porous perovskite heterojunction, and long-term aging tests over 1000 hours confirmed the enhanced stability of the PDPPDBTE-based cells.

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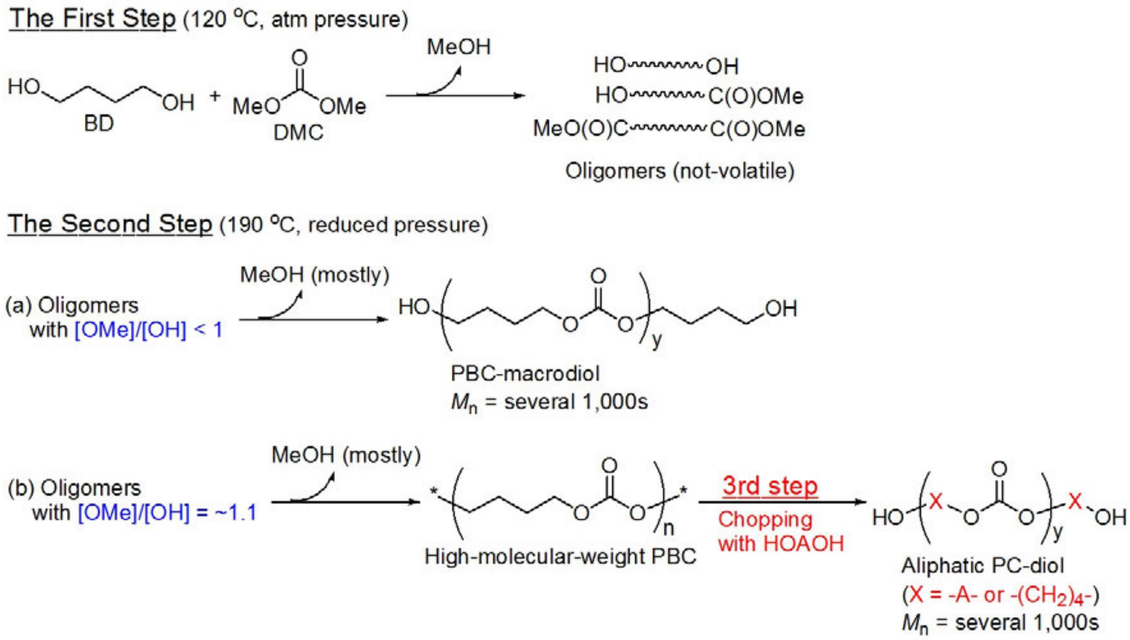
Preparation of Macrodiols and Polyols from Aliphatic Polycarbonates

황은영 이분열[1,*]

아주대학교 분자기술학과 [1]아주대학교 분자과학기술학과

Polyurethanes are used in a wide array of areas. Viscous, oily macrodiols or polyols react with diisocyanates to form PUs. Most of all, Aliphatic polycarbonate-based macrodiols or polyols have some merits. These are not as hydrolytically unstable as the polyester-based ones, and show high resistance against sun-light and oxidative degradation. In addition, Theses include improved antistatic effect and biocompatibility. Despite aforementioned merits, theses are being used on a limited scale because of relatively high preparation cost. So we report an efficient synthetic strategy. High-molecular-weight poly(1,4-butylene carbonate) was prepared through the condensation polymerization of dimethyl carbonate and 1,4-butanediol in the presence of 0.05 mol % sodium alkoxide catalyst. The subsequent feeding of 15 mol % HOAOH, such as 1,6-hexanediol, glycerol propoxylate and stirring at 190-150℃ converted the extremely thick high-molecular-weight polymer to low-molecular-weight macrodiols with GPC-measured Mn ~2000. In the presence of the sodium alkoxide catalyst, a reversible transesterification occurred between the carbonate group in the polymer backbone and hydroxyl group either in HOAOH or the generated chain end, along with a reversible rapid proton exchange reaction. The H-NMR spectra indicated that the DPs of the resulting macrodiols were well controlled by the mole of the fed chopper. Moreover, the randomization of the repeat units was nearly reached. When the chopped polymers were genuine PBCs, the resulting macrodiols or polyols were in a waxy state at room temperature. However, permanently oily compounds were obtained when the chopped polymers were prepared using 0.90 mole fraction of BD admixed with various other diols.

Scheme 1. Strategies for preparation of aliphatic polycarbonate-based macrodiols.



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Synthesis of Silica Hollow Composite Particles

정종언 이동훈* 김동현 진정운

위덕대학교 그린에너지공학부

A facile and effective approach has been developed to prepare hybrid hollow microspheres by a pickering miniemulsion polymerization method. Using the colloid as a sacrificial core, the resulting composites could be converted to hollow spheres by selectively removing the polymer cores by calcinations. The hollow composite particles were characterized by dynamic light scattering (DLS) and scanning electron microscopy(SEM).Keywords: hollow particles, core-shell particles, emulsion copolymerization, composite particles.

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P-type Conjugated Polymers Based on 2,2’-(1,2-ethenediyl)bisthiophene and Dithieno[3,2-b;2’,3’-d]thiophene Units for High Performance Organic Field Effect Transistors

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Conjugated polymers based on thiophene unit have been studied for years in organic electronics because of its highly electron rich and moderate charge transport characteristics. Polythiophenes containing rigid and planar backbone, in particular, have been known to show relatively high charge carrier mobility due to their superior pi-orbital overlap property. Recently, 2,2’-(1,2-ethenediyl)bisthiophene (TV) and dithieno[3,2-b;2’,3’-d]thiophene (DTT) units are widely used for such purpose that vinyl group and fused thiophene structure prevent angular torsion of conjugated structures. In this presentation, we copolymerize TV with DTT unit to yield high mobility conjugated polymer, PTV-DTT. With this polymer, hole mobility exceeding 3 $cm^2V^{-1}s^{-1}$ was achieved in top gate/bottom contact OFET devices and this is the highest record for all-thiophene based polymers that have ever published. Overall characterization of the polymer including UV-Vis absorption, cyclic voltammetry, x-ray diffraction measurement and molecular modeling were performed to figure out the reason for high charge carrier mobility of the polymer in respect of structural perspective.

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Alkylated Thienylenevinylene and Benzotriazole based Donor-Acceptor Copolymers for Organic Thin Flim Transistors

이민혜 김동유[1,*]

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

π-conjugated polymeric materials have emerged as promising semiconductors for solution processable organic optoelectronic applications, such as organic thin-film transistors (OTFTs). Designing Donor-Acceptor copolymers, which provide extended π-π overlap in ideally more than one spatial direction and enhanced intramolecular charge transfer, is one of facile approaches for high performance OTFTs. Among recent researches, organic devices using Poly(thienylene vinylene) (PTVs) units showed high charge-carrier mobility due to high degree of crystallinity with close π-π stacking facilitating planarity. Improved solubility and molecular ordering were also observed in alkyl substituted PTVs. As electron-acceptors, Benzotriazole (BTz) units are one of the promising candidates since both modification of the N-H bond of BTz units and synthesis are facile. For those reasons, two types of BTz units with linear and branced alkyl chain were copolymerized with alkylated thienylenevinylene (TV) by stille polymerization. The polymer based OTFTs were fabricated as top Gate-Bottom contact structure. The devices showed high field-effect hole mobility of 1.9 cm^2/Vs.

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Effect of End-groups on Photovoltaic Property of Pyrazole Substituted Thiazolothiazole Derivatives

임대희 장수영 김동유[1,*]

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Bulk heterojunction organic solar cells based on blend system of electron donor and electron acceptor for active layer are receiving extensive academic and commercial interest. In case of small molecule donors, they have advantages of relatively simple synthesis, high reproducibility, easy purification and high molecular weight precision compared with polymers, however, their low viscosity causes a problem of film formation due to their low intermolecular interaction. Among lots of donor materials, thiazolothizole has a rigid and coplanar fused ring, and thereby ensures highly extended π-electron system and strong π-π stacking. In this presentation, we demonstrate the synthesis and characterizations of thiazolothiazole derivatives including pyrazole end-group for improvement of intermolecular interaction using hydrogen-bonding. The molecular structure and their optical, thermal and electrochemical properties were investigated.

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Synthesis of Urea using CO_2 Chemistry

김유진 김상율*

한국과학기술원(KAIST) 화학과

Urea derivatives are useful chemical intermediates in the synthesis of pharmaceuticals, agricultural chemicals and dyes; and they were also used as antioxidants in gasoline and additives in plastics. Conventional preparative methodologies of urea derivatives are based on the used of dangerous reagents such as phosgene and isocyanates. Replacement of these hazardous reagents in chemical processes is one of the main goals in green chemistry. Therefore, the synthesis of ureas starting from CO_2 has drawn much attention because CO_2 is a renewable, abundant, cheap, and nontoxic source of functional carbon unit.We report synthesis of urea compounds starting from cyclic carbonates which are derived from CO_2 and epoxide. Various Structural modification was attempted to study its outcomes.

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Hybrid Hierarchical Nanostructures for Alternative Electrodes in Dye-Sensitized Solar Cells

QUAN LINA 김동하*

이화여자대학교 화학나노과학과

The electrode in dye-sensitized solar cells (DSSCs) demands high porosity and surface area so that the sensitizers can be sufficiently adsorbed and the paths for electron transport can be electronically interconnected. Highly ordered hierarchical mesoporous TiO_2 networks can provide fast electron transport paths, and ordered mesopores can enhance light scattering, facilitate infiltration of the electrolyte, and ultimately increase the power conversion efficiency. In this work, we investigated the formation of hierarchical mesoporous TiO_2 and carbon-TiO_2 nanostructures and their application as photoanode in DSSCs. Those structures were fabricated by using polystyrene beads for SiO_2 inverse opal template, and infiltration of a common solution consisting of amphiphilic triblock copolymer (P123) and TiO_2 sol-gel precursors. A commercially available triblock copolymer Pluronic P123 played key role in the generation of nanovoids within the hierarchical mesoporous TiO_2 opal and also as a carbon source. Mesoporous carbon-TiO_2 opal is fabricated via sequential UV-stabilization and calcination of P123 containing TiO_2 precursors and their performance as electrode was compared with carbon-free analogues. The changes in photovoltaic performances were monitored by controlling the loaded amount of mesoporous TiO_2 opals and carbon-TiO_2 opals. It was observed that the incorporation of mesoporous carbon-TiO_2 opals into the conventional photoanode of DSSCs can enhance the charge transport and collection that lead to enhanced photovoltaic performance by ~25.78 %.

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Condensation polymerization of high-molecular-weight poly(1,4-butylene carbonate-co-terephthalate)and its thermal properties

어성찬 이분열*

아주대학교 분자과학기술학과

Social demand is increasing for biodegradable and compostable polymers. Annually, mankind produces more than 200 million tons of polymers, almost all of which are persistent in the ecosystem and create disposal problems. Aliphatic polyesters have drawn attention as compostable alternatives for persistent petroleum-based polymers. PHA and PLA, currently on the market, are produced from renewable resources using microbes or fermentation. Poly(1,4-butylene adipate-co-terephthalate) (PBAT) was recently commercialized and has drawn a lot of attention. Even though it contains aromatic units in significant amounts, it was reported to be totally compostable without environmental risk. Aliphatic polycarbonates are also reported to be biodegradable. High-molecular-weight PBCTs with varying terephthalate contents were prepared with Mw 60000-200000 by the condensation copolymerization of BD, DMC, and DMT. The polymerization could be easily performed using inexpensive NaOH (0.1-0.2 mol%) as a catalyst in a reasonably short reaction time, totaling 8.5 h, and on large scale. Attractively, the prepared PBCTs bearing 40-50 mol% terephthalate units showed thermal properties comparable to the compostable aliphatic polyesters currently available on the market (PLA, PHA, PBAT, and PBSA). Melting temperatures were observed in the range 95-146℃, which could be modulated by the terephthalate content, with a fast crystallization rate. Because the monomers (BD, DMC, and DMT) are inexpensive chemicals produced annually on bulk scale, PBCTs may have the potential for commercialization. In terms of its chemical structure and thermal properties, PBCT is similar to PBAT, but they feel different to the touch. PBAT is somewhat sticky and PBCT is not.

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발표종류: 포스터, 발표일시: 수 16:00~19:00

Formation of catalyst-free hydrogels by interfacial chemical activation of immobilized catalysts

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한국과학기술원(KAIST) 화학과

Hydrogels are an attractive biomaterial for use in tissue engineering, drug delivery and macromolecule biosensors. Important aspects to be considered during the preparation of hydrogels are controllable crosslinking and excellent biocompatibility. In formation of controllable in situ hydrogels, covalent crosslinking chemistry using biological or chemical catalysts have been utilized. However, for the chemically crosslinked hydrogels, chemical catalysts such as copper(I) salts NaIO4, FeCl3, or enzyme are unavoidably incorporated into the hydrogel. This might cause a possibility of unexpected toxicity in the human body, which includes a series of toxicological evaluation. Accordingly, the most challenging problem has been recognized in terms of catalyst incorporation. In this study, we introduce an entirely new method to form hydrogels, whose formation is triggered by a catalyst, but the resulting hydrogels are catalyst-free due to immobilization of catalysts on portable surfaces. Therefore, we chose the catechol-containing polymer and hematin as a model of a hydrogel preparation method. Catalytic activity of the surface-immobilized hematin converts catechol to crosslinkable quinone/semiquinone free radical resulting in formation of hydrogels. However interestingly, we found that the chemically active radicals are effectively generated by simple contact with surface-immobilized hematin. Action of the surface-immobilized hematin results in kinetically controlled crosslinking that eventually forms catalyst-free injectable hydrogels.

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발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis and characterizations of naphthalene and phenanthrene polymer derivatives for organic electronics

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Over the past 10 years, extensive research has been conducted about organic electronics, particularly organic solar cells (OSCs) and organic thin film transistors (OTFTs), due to their light-weight, cheap, flexible properties. To attain the high device performance, research on new materials for photoactive layers and semiconducting layers has received a lot of attention. Conventional polythiophene derivatives such as regioregular poly(3-hexyl thiophene) (rr-P3HT) is a promising candidate as an electron donor for bulk heterojunction (BHJ) OSCs, but PCE of rr-P3HT has been limited by low open circuit voltage (Voc) and limited photon absorption at the long wavelength region. Our approach to achieve better performance is to increase Voc by introducing fused benzene ring based polymers as donor materials for OPVs. Naphthalene and phenanthrene are two kinds of the fused benzene ring compounds and they have chance to achieve higher Voc due to their deeper HOMO level than that of thiophene derivatives. Moreover, their rigid planar structure has potential for high mobilities. We used a diketopyrrolopyrrole (DPP) unit as an electron accepting moiety for donor-acceptor type alternating copolymers for reducing the optical band gap. In this presentation, we will report the material synthesis, characterization, and device performance of these novel low band gap polymers.

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

Nano-assembly based on host-guest chemistry for delivery of nitric oxide

강영남 김원종[1,*]

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While most of the studies have heavily concentrated on demonstrating the versatility of the nitric oxide (NO) releasing materials, little effort has been spared to develop successful NO-delivery strategies for advancing NO-mediated therapy. Therefore, development of a rational NO-delivery system has been one of the significant issues in biomedical applications of NO. Herein, we describe a novel supramolecular nano-assembly formed by multivalent interaction between cucurbit[6]ril conjugated dextran (CB[6]-Dex) and diazeniumdiolates-spermine conjugated dextran (NONOates-Spm-Dex). This nano-assembly not only showed the sustained NO release due to its hydrophobic environment by allyloxy group, but also demonstrated the great stability of nano-assembly due to the multivalent host-guest interaction. This novel system is expected to offer versatile tools for various biomedical applications such as wound healing, anti-restenosis, anticancer and antibacterial agent.

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Fabrication and Characterization of Single Crystalline TiO_2 Nanowires

김지태 김희수 박순천 정광운[1,*]

전북대학교 고분자나노공학과 [1]전북대학교 고분자.나노 공학과

Epitaxially grown titanium dioxide (TiO_2) nanowires containing single crystalline TiO_2 nanofibers with anatase structure were fabricated by electrospinning poly(vinylpyrrolidone)/ethanol solutions mixed with hydrothermally synthesized titanium dioxide nanowires and titanium (Ⅳ) isopropoxide precursor. Utilizing Scanning Electron Microscope(SEM) and High Resolution Transmission Electron Microscope(HR-TEM), morphological examination was conducted. Structure and orientation of TiO_2 single crystalline nanowires were also identified by XRD and SAED simultaneously. Improved optoelectronic properties of TiO_2 nanowires were also identified with UV-Vis spectroscopy experiments. This work was mainly supported by the Human Resource Training Project for Regional Innovation and the Converging Research Center Program (2013K000404) of Korean government.

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발표종류: 포스터, 발표일시: 수 16:00~19:00

DNA conjugated cyclodextrin polyrotaxane nanoconstruct for targeted and stimuli-responsive drug delivery

장동현 김원종*

포항공과대학교 화학과

A cyclodextrin (CD) polyrotaxane (PR) structure was synthesized as a targeted and stimuli responsive drug delivery carrier. A DNA aptamer (DNA_a), *i-motif* DNA (DNA_i) and its complimentary DNA ($cDNA_i$) were each conjugated to α-CD. These 3 types of CD-DNAs formed a pseudo-PR with diaminopolyethylene glycol ($PEG\text{-}AM_2$) by simple sonication. Here, one pseudo-PR contained $CD\text{-}DNA_i$ and $CD\text{-}DNA_a$, while another had $CD\text{-}cDNA_i$ and $CD\text{-}DNA_a$. Finally, both ends of $PEG\text{-}AM_2$ were capped with 1-Fluoro-2,4-dinitrobenzene to yield two different PRs. By annealing *i-motif* PR and its complimentary PR, a DNA crosslinked nanoconstruct had been formed. Doxorubicin, a well-known anticancer drug, was intercalated between the double-stranded DNA and released by the formation of *i-motif* structure in endosomal pH condition. Targeting ability was introduced by cancer cell specific aptamer sequence of $CD\text{-}DNA_a$, which was threaded to PEG with either $CD\text{-}DNA_i$ or $CD\text{-}cDNA_i$. With easily replaceable targeting moiety by modular design and controllable drug loading capacity by altering feed ratio, this system will enable patient-specific treatment with active targeting ability in a stimuli-responsive manner.

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Paclitaxel Delivery System Based on Multivalent Host-Guest Interaction of Poly-Cyclodextrin and Poly-Paclitaxel for In Vivo Cancer Therapy

장유나 이영민* **Allan S. Hoffman**[1,*] 김원종*

포항공과대학교 화학과 [1]University of Washington, USA

Paclitaxel (PTX) is one of the most effective chemotherapeutic drugs used to treat various cancers such as breast, ovarian, lung, head and neck cancers. However, its therapeutic potential has been severely hampered by its poor solubility in water and physiological conditions. To surmount these issues, herein, we developed a novel self-assembled inclusion complex through host-guest interaction between PTX and cyclodextrin (CD). CDs are cyclic oligomers of α-1,4-D-glycopyrianoside, a cup-shaped molecules with a hydrophilic exterior and an internal hydrophobic cavity. CD and PTX are covalently conjugated to biodegradable poly(maleic anhydride) backbone via an ester linkage. The self-assembled inclusion complex formed nano-sized particles of size less than 100 nm. It resulted in a significant increase in PTX water solubility than free PTX. Furthermore, this inclusion complex showed enhanced antitumor effect than free PTX. This novel self-assembled PTX-CD inclusion complex has high potential as a controlled drug delivery system for PTX in cancer therapy.

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Bio-inspired polydopamine capsule for delivery of nitric oxide

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포항공과대학교 화학과

The paramount biological roles of nitric oxide (NO), such as angiogenesis, apoptosis, immune response, neurotransmission, and cardiovascular homeostasis, have spurred many researchers on efforts to develop diverse NO-delivery systems. Nevertheless, the day when developed NO-based drugs can be applied to real clinical therapy is still far-off. Herein, we describe a bio-inspired polydopamine (pDA) capsule-based NO delivery platform for echogenic diagnosis, antibacterial application or anticancer therapy. The pDA capsule is developed by the spontaneous oxidative polymerization of a dopamine onto silica (SiO_2) particles, followed by removal of the template particles. To develop the pDA-NO capsule, NO is stored not only onto the pDA film layers by the formation of diazeniumdiolates, but also into the hollow space of pDA capsule as a gas state. The possibility of pDA-NO capsule on bioapplication has been under way.

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Self-polishing copolymer based on ZnMA monomer containing Acrylic resin using Radical polymerization

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Anti-fouling are used to prevent the growth of marine organisms on the bottoms of ship’s hulls. These organisms have extremely adverse effects on both speed and fuel consumption. Zinc containing Acrylic or methacrylic copolymers are easily hydrolyzed in seawater. Fouling organisms, which attach on the surface of a paint film, can be eliminated together with the copolymer film by the hydrolysis of the copolymers.In this study, Zinc methyl methacrylate (ZnMA) by using zinc oxide and Methacrylic acid (MAA) was synthesized. And then we used ZnMA and acrylic monomers to develop self-polishing copolymer (SPC). Synthesis and properties of zinc containing resin were investigated by 1H-NMR, gel permeation chromatography (GPC), inductively coupled plasma (ICP) mass and infrared (IR) spectroscopy. The polishing rate was determined by measuring the film thickness after a dynamic immersion test.

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IR 과 MALDI를 이용한 TDI와 TMP의 반응 조성물 분석에 관한 연구

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순천향대학교 화학과

Acrylic Polymer 제조시 사용되는 경화제는 isocyanate 와 polyol 로 구성되어 있다. 본 연구에서는 이 중 대표적인 화합물인 toluene diisocyanate(TDI)와 trimethylolpropane(TMP)를 반응 시키고 반응진행 과정을 infrared(IR) absorption spectroscopy 과, Matrix-assisted laser desorption/ionization mass spectrometry(MALDI MS)로 추적하였다. 각각 다른 TDI/TMP 의 비율을 이용하여 다양한 반응을 확인하였으며, 시간경과에 대한 polymerization 반응 진행 정도는 IR 을 이용하여 확인하고, MALDI MS 를 이용하여 polymer product 의 상대적인 composition 과 결과를 추측하고 확인하였다. IR 과 MALDI MS 를 이용하면 시간 경과에 따른 polymer 의 composition 을 실시간 monitoring 이 가능하다.

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Selective Ethylene Oligomerization with Chromium Phenylene-Bridged SNS Catalytic System

정태욱 김상율*

한국과학기술원(KAIST) 화학과

1-Hexene and 1-octene are very important and highly demanding comonomers used for the synthesis of linear low-density polyethylene (LLDPE). But they are mainly produced by conventional ethylene oligomerization process like Shell Higher Olefin Process (SHOP), which yield a full range of linear α-olefins based on Schultz?Flory distribution, and have to be isolated through inefficient process. Therefore, a lot of effort has been devoted to achieve a selective tri- or tetramerization of ethylene. McGuinness and coworkers reported that tridentate SNS systems showed the high selectivity of 1-hexene and good activity. In this study, we conducted the ethylene oligomerization with phenylene-bridged SNS Cr catalyst to investigate the effect of temperature, lignad structue, run time and ethylene pressure.

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Microcapsulation of High Contrast Quasi-Amorphous Photonic Solutions for Photonic Applications

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Colloidal nanoparticles have been extensively investigated as a fundamental tool for understanding crystallizations and as an building block for novel functional materials. QAPS(Quasi-amorphous photonic solutions) have been received many attention because it exhibits angle-independent and non-brilliant photonic color. QAPS exhibiting high color saturation and color gamut were prepared by using SiO_2 nanoparticles modified with polydopamine (PDA). The QAPS can be encapsulated into uniform double emulsion type microcapsules by using multi-channel microfluidic device. These results for high contrast of capsulated QAPS may pave the way toward developing practical applications of photonic display pixels.

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A colorimetric sensor for identification of toxic gases

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Colorimetric gas sensor system has been developed to identify the presence of toxic gases.The commertially available sensing system that employ electrochemical cell suffer poor selectivity, high power consumption, long term stability and are expensive. To overcome these drawbacks of the existing technology, we have developed colorimetric nano fiber sensors by electrospinning for detecting toxic gases such as HF, HCl, Cl_2, NH_3, HCHO, N_2H_4, CH_3NH_2, SO_2, $(CH_3)_3N$ and NO_2. We demonstrate that our fluorescence dye nano fiber system is highly sensitive and selective. As an important application of our sensor system, we selected coumarin based organic molecules and dye. We synthesized a coumarin derivatives with varying electron-donating groups in the 7-position of the coumarin to tune the absorption and emission wavelengths. The structure of synthesized organic molecules and nano fiber are characterized with by NMR, optical microscopy, UV, PL, SEM.

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Synthesis of cabazole-based acceptor-donor-acceptor type conjugated molecules for organic solar cells

류바울 박상혁*

공주대학교 화학과

Organic solar cells possess many benefits such as low cost, mechanical flexibility, light-weight, and facile fabrication for large area. One of the most important issues is the improvement of power conversion efficiencies (PCEs) in actual solar cell devices. To resolve this low PCE according to the absorption limitation, we have synthesized new low bandgap molecules consist of D (electron-donating unit) and A (electron-accepting unit) alternative structure (A-D-A) with carbazole derivatives. In this work, the synthesis and their optical and electrochemical properties will be presented along with their application to organic solar cells.

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DPP-based Donor-Acceptor Alternating Copolymers containing Benzo[1,2-b;4,5-b’]dithiophene and Anthracene-based Monomers for Organic Photovoltaic Cells

홍한나 이대희 엄현아 신지철 조민주 최동훈*

고려대학교 화학과

Bulk-heterojunction (BHJ) solar cells with the blending of donor-acceptor (D-A) polymers based on solution-processible fabrication have been broadly researched because of promising advantages such as light weight, cost-effective manufacturing, and the possibility of flexible large-area devices for future industrial applications. Various conjugated polymers containing diketopyrrolopyrrole (DPP) in the repeating group were reported in the literature for showing their superb electronic device applicability. In our previous work, we reported DPP based polymers bearing benzo[1,2-b;4,5-b’]dithiophene (BDT) and anthracene (Ant) as donor units, P(DPPBDT) and P(DPPANT), for which we obtained favorable hole mobility of 1.14 and 1.90 cm^2 V^{-1} s^{-1}. These copolymers were highly crystalline and provide very promising charge transport property. For these reasons, we tried to fabricate polymer solar cell devices with well-known PCBM as an acceptor.

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Synthesis and Structure-charge Transport Property Correlation of Diketopyrrolopyrrole-based conjugated Polymers

최수나 박지은 신지철 조민주 최동훈*

고려대학교 화학과

Diketopyrrolopyrrole (DPP)-based conjugated donor-acceptor (D-A) copolymers containing fused-aromatic ring as a donor unit have received a great attention recently. Among them, fused-aromatic moeity-bearing copolymers showed much higher charge carrier mobility due to strong stacking interaction. In this presentation, we demonstrate the synthesis of new DPP-based copolymers containing naphtho[1,2-b:5,6-b′]dithiophene (NDT) and benzodithiophene (BDT) as donor units. These copolymers having highly crystalline structure can be expected to show promising charge transport phenomenon. Therefore, we try to investigate their physical properties by thermal analysis, cyclic voltammetry and absorption spectroscopy. As a result, we successfully fabricated field-effect transistor devices to compare their charge transport properties.

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Preparation of $H_3Co(CN)_6$ Using Ion Exchange Resin for Highly Active Double Metal Cyanide Catalyst

박동식 이분열*

아주대학교 분자과학기술학과

Abstract: Low molecular-weight poly(propylene oxide-co-propylene carbonate)-diols was used in polyurethane industry. Diols having carbonate linkage of 65% and average molecular weight (Mn) 2000 g mol^{-1} can find suitable place in polyurethane industry. As the new Double metal cyanide catalyst is working well with wide range of carboxylic acids as chain transfer agents, low MW poly(PC-co-PO)-diols can be prepared by addition of various carboxylic acids. These promising diols were used in preparation of polyurethane. The preparation method of catalyst includes by removing K^+ ions at the initial stage. 30-35 % ether linkage give flexibility to polymer backbone.

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Fabrication of Dually Functionalized Surfaces on an Au Substrate Using a Si-Containing Block Copolymer and Their Applications

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한국과학기술원(KAIST) 화학과

Chemical surface nanostructures were obtained using self-assembled monolayers patterned by microcontact printing or nanoimprint technique. But these approaches are inadequate at the micron- and sub-micron scales. Serial techniques like dip-pen and electron-beam lithographies achieve nanoscale pattern definition but are limited in their ability to define large area patterns. In this study,Si-containing block copolymers were used for fabricating highly ordered nanoporous SiO_2 structures on a gold substrates. The substrate was chemically and topographically patterned to give silicon oxide and gold surfaces. The two types of surfaces allow two different chemical functionalities, in this case, silane and thiol compounds, to be reacted to silicon oxide and gold surfaces, respectively. This dually patterned self-assembly method not only forms ordered nanostructures over large area, but also controls surface property by changing functional groups of self-assembled molecules. These dually patterned surfaces would be further utilized for immobilization materials such as nanopaticles, DNA, and proteins. This patterning technique can be highly useful for the high throughput biosensor and array applications.

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Synthesis and characterization of Polythiophene-like films by PECVD

정동철 송선구 최은정 송창식*

성균관대학교 화학과

Applications of polythiophene semiconductors or conducting films have been widely explored in transistors, solar cells, light emitting diodes (LEDs) and sensors. The polythiophene family has been conventionally synthesized by either electrochemical or chemical methods. However these kinds of methods have drawbacks such as difficulties in processing in large scales and substrates limitations. Moreover, While producing the substrates could be destroyed due to poor mechanical property of the substrates. Plasma polymerization is a room-temperature, solvent-free and catalyst-free process that polymers can be rapidly deposited on various surfaces. It could form high degree of cross-linking films and easily control the thickness of films. In this study, Plasma-polymerized polythiophenes were deposited as thin films utilizing plasma of mid-range frequency (40 kHz) and low power (4W). The thin films were prepared by changing the distance from the top electrode to the substrates, and the resulting films were compared. Conductivity increased with distance up to 110 mm, and then decreased with further increase in distance. FT-IR and XPS analysis showed that the thin films had similar molecular structures regardless of the distance. However, as the distance increased, surface roughness increased from 0.54 to 5.53 nm, which suggested gas-phase nucleation and molecular packing.

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Synthesis of fluorinated alkyl benzothiadiazole-based donor-acceptor molecules for organic photovoltaic cells

이은혜 박상혁*

공주대학교 화학과

Organic photovoltaic (OPV) devices are important candidates for future energy sources due to their light and flexible characteristics. However, efficiencies of OPV devices are generally lower than silicon based solar cells. In this work, to enhance power conversion efficiency, fluorinated benzothiadiazole substitution were designed and synthesized. The fluorine atom (F) is effective electron withdrawing unit, and the introduction of F can lower LUMO and HOMO energy levels in common donor-acceptor type conjugated molecules. Also, alkyl group was introduced in the fluorinated benzothiadiazole unit to enhance solubility to organic solvents. In this study, we will present the effect of fluorinated benzothiadiazole derivatives for solubility as well as solar cell efficiency enhancement.

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Synthesis and characterization of PVA hydrogel thin film for drug delivery application

KHALEELZINAHHILALKHALEEL 최은정 차인환 송창식*

성균관대학교 화학과

Hydrogel is hydrophilic polymer, capable of containing large amount of water. Hydrogel materials consist of water-swollen polymer networks. Hydrophilic groups such as hydroxyl and carboxyl their back bonds absorb and store water, We made hydrogel film using Cupper-Azide-Alkyne cycloaddtion (CuAAc) by generating Cu(I) electrochemically which is required to complete between alkynes and azides at room temperature. We worked on optimizing the conditions to control the film thickness and weight with and without CNT and thickness of film measured using alpha-step and weight measured using Quartz Crystal Microbalance (QCM). The aim of this research is to get a thin hydrogel film which can be use in drug releasing system as a patch or inject inside the body.

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Synthesis and characterization of hydrogel system furnished electro-conductivity

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성균관대학교 화학과

Electro-conductive hydrogel is a polymeric blend or co-network that combines electro-active molecules, including conducting polymers, with hydrogels.1 Such hydrogel-polymer hybrid material has the electrical properties with electro-active molecules, 3-dimensional framework and highly hydration. In this study, HA-DOPA hydrogel was synthesized by crosslinking using dopamine linker, and the properties of HA-DOPA hydrogel are tuned with adding electro-active molecules like carbon nanotubes or polypyrroles. The electro-active molecules improve the electro-conductivity and the strength of hydrogels. Moreover, the properties of hydrogel could be improved when electro-active molecules make better co-networks with hydrogel. Electro-conductive hydrogel system may act as an electro-stimulated drug release system.

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Conductive Polymer/Polydopamine Capped Graphene Oxide Nanocomposites for Supercapacitors

차인환 이윤미[1] 안종호 이지영 박선화 송창식*

성균관대학교 화학과 [1]광운대학교 화학과

Supercapacitors have been highlighted as the next generation energy storage devices due to fast charge/discharge rate, high efficiency, and semi-permanent characteristics. Conductive polymers are used as electrode materials and they have some advantages differentiated such as flexible, eco-friendly, safety and low cost than inorganic materials. Dopamine, one of the bio-molecule, have catechol moiety that helps additional capacitance by redox reaction from catechol to quinone. We report a new nanocomposite based on polydopamine (PDA)-capped graphene oxide (PDA-capped GO) and 3,4-ethylenedioxythiophene (EDOT). Because PDA-capped GO have catechol moiety by polydopamine, so we predict more capacitance than graphene oxide (GO). PDA-capped GO and PEDOT nanocomposites were prepared from one?step coelectrodeposition. During the process of electrochemical polymerization, the anionic PDA-capped GO acted as a weak electrolyte and was entrapped in the conductive polymer nanocomposites. We investigated morphology by SEM image and electrochemical properties such as cycling performance, capacitance and impedance of PDA-capped GO/PEDOT polymer nanocomposites, and compared with those characters of GO/PEDOT nanocomposites.

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Synthesis and characterization of N-heterocyclic carbene conjugated polymer and gold nanoparticle hybrid material

송선구 정동철 최은정 송창식*

성균관대학교 화학과

Polymer-nanoparticle composite materials for several devices have been studied due to its mechanical, electrical, optical and thermal properties. We synthesized Gold nanoparticles and N-heterocyclic carbene(NHC) conjugated polymer hybrid materials expecting that conjugated structure could make better electron transfer from the metal nanoparticle part. In this system, disproportionation of gold attached to the NHC makes Au(0) and Au(III). Au(III) oxidizes the end group (bithiophene) and makes the conjugated polymer with NHC. This NHC-conjugated polymer stabilizes the gold nanoparticles made from Au(0). This nano-aggregate products were characterized by XRD, TEM and solid state NMR to find the interaction between gold nanoparticle and conjugated polymer. We can use the gold nanoparticles to water splitting process which helps suppress back-reaction which makes water from hydrogen and oxygen gas and improve the efficiency of water splitting. And also the electron accepting molecules (like C60) improve the efficiency of water splitting. Hence, we design the functionalized the NHC ligand group to find out whether the efficiency will be improved through the conjugated structure and electron accepting group.

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Irreversible sealing of plastics with elastomer via one-step room temperature surface modification

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가천대학교 글로벌캠퍼스 바이오나노학과 [1]가천대학교 바이오나노학과

In this study, we introduce a simple and facile strategy for bonding various plastics with transparent elastomer, poly(dimethylsiloxane) (PDMS), via one-step surface modification at room temperature. Here, various plastics such as polycarbonate (PC), polyethylene terephthalate (PET), polyvinyl chloride (PVC), and polyimide (PI) were bonded irreversibly with PDMS by treating the surfaces of plastics with amine-PDMS linker at room temperature for 20 min. In this way, the carbon backbone of the plastics reacted with the amine functionality of the amine-PDMS linker by forming robust urethane bond. This resulted in the PDMS functionality being exposed on the plastic surface, mimicking the surface of plastics like that of bulk PDMS. After surface oxidation of both surface-modified plastics and PDMS, they came into conformal contact with each other and were thermally cured at 80C for 60 min. In this way, permanent siloxane bond (Si-O-Si) was formed between the plastics and PDMS. The bond strengths of PC, PET, and PVC with PDMS were measured to be approximately 428.5 ± 17.9, 361.7 ± 31.2, and 430.0 ± 14.9 kPa, respectively. The bond strength of a PC?PC homogeneous assembly was measured to be approximately 343.9 ± 7.4 kPa.

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Selective surface modification of a substrate for targeted immobilization

WUJING 이내윤[1,*]

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In this study, a simple and rapid method to endow both hydrophobic and hydrophilic surfaces on a single substrate was demonstrated and applied for a targeted adhesion of functionalized beads. Microwell-patterned polymer substrate was fabricated using a photocurable prepolymer, and while the surface of the replica was partially cured, it was contact printed with a flat, hydrophobic poly(dimethylsiloxane) (PDMS) elastomer, and the assembly was further cured under UV for approximately 3 h and detached. In this way, the PDMS molecules were transferred selectively onto the protruding regions of the partially-cured microwell-patterned substrate, while the inner walls of the microwells remained hydrophilic. As a practical application, functionalized polymer beads were successfully targeted into arrays of microwells without being adsorbed onto the protruding regions of the microwell-patterned substrate. This will pave the ways for targeted immobilization of biomolecules with high selectivity in a relatively simple and facile manner.

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Hydrophilic surface engineering of polycarbonate for genetic analysis

ZHANGYU WUJING 이내윤[1,*]

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In this paper, we introduce a simple strategy for modifying the surface of polycarbonate (PC) hydrophilic. Aminosilane bearing a secondary amine was used, and a strong urethane bond was formed via aminolysis of the carbonate backbone of the PC, leaving alkoxysilane parts exposed on the surface. In-depth surface characterizations were performed, including water contact angle measurement and X-ray photoelectron spectroscopy (XPS) analysis, in order to identify the optimum conditions for achieving hydrophilic PC without sacrificing substrate transparency. To extend the concept of surface modification of PC to microfluidic application, the hydrophilic coating was further adopted in bonding two PC substrates by forming Si-O-Si bonds at the interface, and the potential of the fabricated PC microfluidic device as a platform for conducting nucleic acid analysis was examined.

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Synthesis of polymeric excipients via nitroxide-mediated radical polymerization for the delivery of cisplatin pharmacophore

권은미 이상민*

가톨릭대학교 화학과

Biocompatible polymers have been proposed as a platform to encapsulate drugs for the selected delivery to disease cells. Although such a delivery system has the potential to decrease the toxic side effects often associated with conventional small-molecule chemotherapy, successes have been limited due to the lack of both targeting ability to a particular diseased site and specific triggers that can release the encapsulated drug under predefined condition. To overcome these challenges, a poly(ethylene glycol)-b-(acrylic acid) has been prepared via nitroxide-mediated controlled radical polymerization, which can then incorporate cisplatin pharmacophore, Pt(II), via the formation of self-assembled polymeric nanoparticles. The resulting particles possess the Pt(II) drug core, where the polymer excipients can be cross-linked via divalent metal coordination that can lead to the enhanced structural stability.

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Donor-Acceptor Alternating Diketopyrrolopyrrole-based Terpolymers and Their Semiconducting Properties

김애선 이대희 엄현아 신지철 조민주 최동훈*

고려대학교 화학과

Recently, diketopyrrolopyrrole (DPP) containing polymers have shown very high hole mobility in thin film transistors (TFTs) and high power conversion efficiency in polymer solar cells (PSCs). Furthermore, pyrene unit have attracted much attention due to strong propensity for π-π stacking in a molecular level and can facilitate the charge transport. In this presentation, we synthesized DPP-based terpolymers bearing different donanting units like pyrene and thienyl unit. These donor units are capable of reducing the energy bandgap between the highest occupied molecular orbital (HOMO) and the lowest unoccupied molecular orbital (LUMO) owing to the extended conjugation length, which is suitable for high-performance PSCs. We performed the analysis of matieral properties by using thermal analysis, cyclic voltammetry and absorption spectroscopy. Consequentially, we investigated their charge transport properties.

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In-Situ Modulation of the Vertical Distribution in a Blend of P3HT and PC60BM via the Addition of a Composition Gradient Inducer

이강영 박태호*

포항공과대학교 화학공학과

2,2,3,3,4,4,4-Heptafluoro-N-phenyl-butyr-amide (F-ADD) was synthesized and shown to induce a composition gradient in a blend of P3HT and PC60BM. The addition of small amounts (ca. 0.5 wt%) of F-ADD modulated the chemical distribution in the blend along the vertical direction by controlling the blend component interface energy through selective interactions between F-ADD and PC60BM. A homogeneous compositional distribution along the vertical direction in the nanostructured bulk heterojunction (BHJ) increased the interfacial area, which shortened the exciton path length to the donor/acceptor interface and improved the photovoltaic performance.

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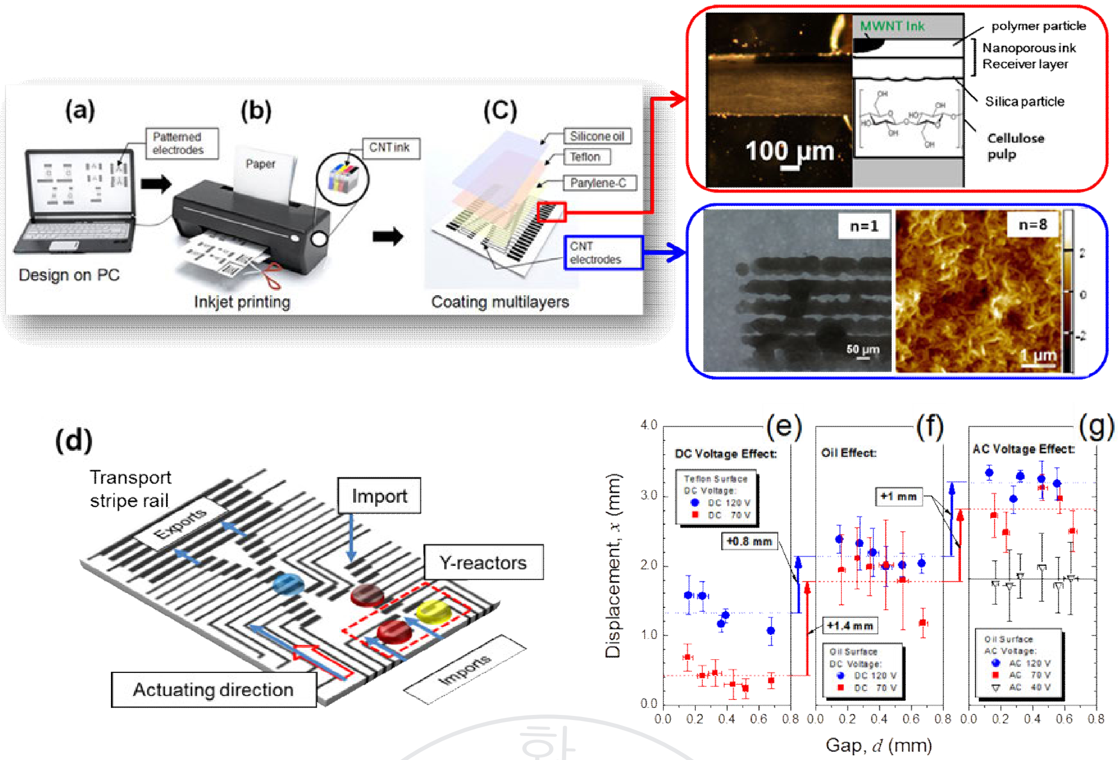
Novel cellulose paper platform for microfluidic lab-on-a-chip printed with CNT ink

김용준 고효진 이주미[1] 김희석 권오선[*] 신관우[2,*]

서강대학교 화학과 [1]서강대학교 화학 [2]서강대학교 화학과 및 바이오융합과정

Cellulose paper, as most aboundent organic polymer in Earth, has been applied for a new platform material for the microfluidic lab-on-a-chip, instead of the conventional substrates such as glass, silicon wafer and polymers. In order to apply the voltage to transport the digitialized drops of liquid samples on paper, a patterned array of electrodes on paper was inkjet-printed with a homemade CNT ink of which viscosity, dispersity and colloidality were treated properly. After depositing dielectric, hydrophobic and low-frictional functional films, the paper chip was realized for the first time. We will present how to enhance the moving distance of drops as a function of two parameters, oil coating and voltage manipulation. It promises the numerous chemical, biological and medical applications, especially as a simple tool for point-of-care diagnosis, which has been arduously demanded in a similar way what litmus, urine and pregnant test paper are ubiquitously used in our daily life.


(a)
Patterned electrodes
Design on PC
(b)
Paper
CNT ink
Inkjet printing
(C)
Silicone oil
Teflon
Parylene-C
CNT electrodes
Coating multilayers
MWNT Ink
polymer particle
Nanoporous ink Receiver layer
Silica particle
Cellulose pulp
100 µm
n=1
n=8
50 µm
1 µm
(d)
Transport stripe rail
Exports
Import
Y-reactors
Actuating direction
Imports
(e)
(f)
(g)
DC Voltage Effect:
Teflon Surface DC Voltage:
DC 120 V
DC 70 V
+0.8 mm
+1.4 mm
Oil Effect:
+1 mm
Oil Surface DC Voltage:
DC 120 V
DC 70 V
AC Voltage Effect:
Oil Surface AC Voltage:
AC 120 V
AC 70 V
AC 40 V
Displacement, x (mm)
Gap, d (mm)
0.0
1.0
2.0
3.0
4.0
0.2
0.4
0.6
0.8

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Microbatch method of protein crystallization for novel microfluidic paper chip platform

김희석 문태우 고효진 김용준 권오선* 신관우1,*

서강대학교 화학과 1서강대학교 화학과 및 바이오융합과정

Microbatch method for protein crystallization has been performed to find out the proper implement way to be realized on the digital microfluidic paper chip platform.[1-3] To satisfy the corresponding path of phase condition for crystallization (the blue thick line in Fig 1a), we controlled the diffusive evaporation rate of water solvent in varying concentration of the precipitant solution (typically, 50 mg/ml lysozyme and 6.5 wt% NaCl precipitant with 0.1 M NaAc buffer of pH 4.8) through a silicone oil reservoir (Fig. 1b). Although there are numerous factors influencing this crystallizing process such as, temperature, protein solution-precipitant ratio, salt concentration and buffer pH, unfortunately there is yet neither a standard guideline or an optimized condition for obtaining just a single protein crystal, especially regarding the oil-depth parameter that is never been before. Here, we investigated the effect of the distance from an immerged droplet to air/oil interface. Consequently, we obtained a good condition for single crystallization around in depth of 1 mm, indicating that this microbatch method using oil depth variation can be used as a very effective way for obtaining the speedy protein crystallization. The results were compared to those of the hanging-drop method (Fig. 1d). Due to the smooth growth trend, the microbatch method should be much suitable for implement of a reactor for a single crystallization on a microfluidic paper chip that we recently developed (Fig. 1e).[4]

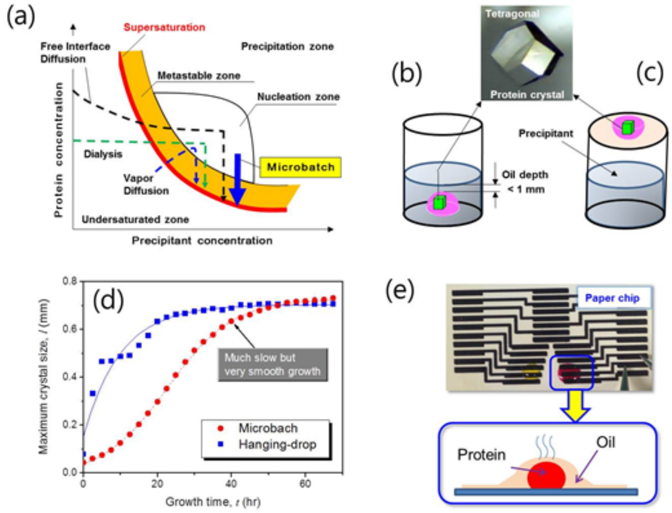

Fig. 1. Protein crystallization to obtain one big single crystal habit: (a) Phase diagram, (b) Microbatch method, (c) Hanging-drop method, (inset) Crystalized lysozyme protein in single crystal in millimeter order and (d) Comparison of the crystal size as a function of time for both methods. (e) Schematic view of crystallization on a microfluidic paper chip using the microbatch method.

Keywords: Protein crystallization, Microbath method, Lysozyme, Microfluidic paper chip.

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Thermogelling polypeptide as a protein drug delivery cargo

SHINDE USHA PRAMOD PATELMADHUMITA 정병문*

이화여자대학교 화학나노과학과

Thermogelling system undergoes sol- to ?gel transition when temperature increases. Poly (ethylene glycol)-poly (alanine-co-phenylalanine) (mPEG-PAF) with different molecular weight of PEG and PAF were synthesized. Sustained release depot of human growth hormone (hGH) was prepared in the subcutaneous layer of rat model by injecting the polymer aqueous solution incorpoated with hGH. One week release profile was confirmed with therapeutic level of 2 ng/mL. In vitro release and stability of hGH were also analyze by HPLC.

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The effect of various contents of a crosslinker mixture on the properties of crosslinked SPEEK membranes using an EB irradiation membrane

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In this study, crosslinked sulfonated poly(ether ether ketone) (SPEEK) membranes were prepared using an EB-irradiation crosslinking method with various content of crosslinker mixture (the weight ratio of 1,4-butanediol divinyl ether to tribally isocyanurate was set to 9/1) and applied as a proton exchange membrane (PEM) for the application of fuel cells. The crosslinked SPEEK membranes were characterized using the gel fraction, chemical stability, dynamic mechanical analysis (DMA), small angle X-ray scattering (SAXS), water uptake, proton conductivity, and sing cell performance.

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Fabrication of nanofiber embedding self-assembled discotic Sunset-Yellow FCF dyes

강동규 김지태 임푸른[1] 최유진[2] 정광운[3,*]

전북대학교 고분자나노공학과 [1]전북대학교 고분자.나노공학과 [2]전북대학교 고분자 나노공학과 [3]전북대학교 고분자.나노 공학과

Chromonic nanofibers with the self-assembled Sunset-Yellow FCF nanocolumns were fabricated by electrospinning method. Based on the thermal, microscopic and scattering experiments, it was verified that Sunset-Yellow FCF molecules formed a glassy columnar nematic (N) phase in the PVP/SSY nanofiber. When the PVP/SSY nanofiber was annealed above the T_g of PVP, the SSY nanocolumns further self-organized into three-dimensional ordered crystals. The uniaxially oriented nanofiber mats embedding assembled nanocolumns may open the new doors for the practical applications of the spun fibers in optical, electronic and optoelectronic devices. This work was mainly supported by the Human Resource Training Project for Regional Innovation, Basic science Research Program (2013R1A1A2007238), Global Ph.D Fellowship Program (2013H1A2A1033907), and BK21 PLUS Program, Korea.

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Gamma ray irradiation effects on fluoropolymer films under various environments

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한국원자력연구소 공업환경연구부 [1]한국원자력연구원 첨단방사선연구소 공업환경연구부

The effects of gamma ray irradiation on fluoropolymer films were invesigated. Samples were irradiated under various environments at room temperature using a gamma ray. FT-IR spectra show that the irradiated fluoropolymer films undergo oxidation by a reaction of radicals generated by irradiation with oxygen in air. The changes in the heat of fusion and the degree of crystallinity of the irradiated fluoropolymers were investigated using DSC, and the results indicate that the chemical structure of the irradiated samples was changed by chain scission and crosslinking reactions. The tensile strength of irradiated fluoropolymer films was found to be decreased, especially when the samples were irradiated under an air atmosphere.

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Preparation and characterization of crosslinked SPEEK/PVA membrane using radiation crosslinking method

우현수 손준용[1] 최재학 신준화[1,*]

충남대학교 고분자공학과 [1]한국원자력연구원 첨단방사선연구소 공업환경연구부

Abstract: Perfluorosulfonate ionomer(Nafion) has many advantages such as excellent thermal and chemical properties and good proton conductivity. However, it has also many disadvantages, such as a high production cost, high methanol crossover, and decreased proton conductivity at temperatures above 80 °C. Therefore, for an alternative to Nafion, many research groups have focused on aromatic hydrocprbon based ion-exchange membranes. Poly(ether ether ketone) [PEEK] has thermal and chemical stability as well as good mechanical properties and a low price. In this study, crosslinked SPEEK/PVA membranes were prepared using an EB-irrdiation method with various contents of PVA. The crosslinked SPEEK/PVA membrane and non-crosslinked SPEEK/PVA membrane were investigated using gel-fraction, IEC, TGA, DSC, and proton conductivity.

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New polymers containing azobenzene group for holographic image recording materials based on photochromic conversion

박정호 박주섭[1] 김인태*

광운대학교 화학과 [1]전자부품연구원 실감정보플랫폼

In this work, new polymers containing azobenzene with electron-withdrawing groups have been designed and synthesized. The polymers were successfully characterized by general organic spectroscopic methods(^{1}H NMR, FT-IR, UV-vis and GPC). Their photo-induced Surface Relief Grating(SRG) formation was produced by exposure to interferenced two coherent laser beams(532nm) in few minutes. This surface of SRG was measured by Atomic Force Microscopy(AFM) image. The diffraction efficiency is observed to less than 1%. The interference pattern of holographic image was illuminated by a green laser at a specific angle and distance on the polymer film. Finally, we successfully obtained a faint holographic image. It can be played back by illuminating with a coherent green laser identical to the reference beam. Due to their properties, we expected that the polymers can be used in various optical data storage devices.

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Donor-Acceptor polymer containing ethylenedioxythiophene and fluorinated benzene derivative for polymer solar cells

장원 김종현 김인태*

광운대학교 화학과

Recently, fluorinated unit in main chain of polymer is interesting in polymer solar cells (PSCs), as its small size is expected to minimize the undesired steric interations and its strong electron-affinity nature is also expected to stabilize the HOMO and LUMO energy levels. So we synthesized copolymer using the fluorinated benzene derivative monomer and 3,?4-?ethylenedioxythiophene (EDOT) monomer. The new polymer was characterized by ^{1}H NMR and IR-spectrum and UV-vis spectroscopy. The properties of the polymer were measured by cyclovoltametry and thermogravimetric analysis. The polymer will be applied to polymer solar cell device.

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Modification of Low Bandgap Polymer using Atmospheric Pressure Plasma Jet (APPJ) with different feeding gases

김영선 김중일 김인태*

광운대학교 화학과

In this poster, we have examined the modification of surface properties of plasma treatment low bandgap polymer using atmospheric pressure plasma jet (APPJ) with different feeding gases. Use of low bandgap polymers is the most suitable way to harvest a broader spectrum of solar radiations for solar cells. But, still there is lack of most efficient low bandgap polymer. In order to solve this problem, we have synthesized and modify the polymer with help of APPJ. Polymer surface modification is an elegant method for generating functional polymer surfaces combined with the desirable attributes of bulk polymers. The use of plasmas for the treatment of solid surfaces has several advantages over conventional solution phase chemistry. Plasma processes are solvent free and energy efficient, rendering them an environmentally friendly and cost effective alternative to traditional methods. Bombardment by energetic particles breaks the covalent bonds at the surface, leading to the formation of surface radicals. The latter can react with the active plasma species to form different chemically active functional groups at the surface. Surface contaminants and weakly bound polymer layers can dissociate into volatile side products, which can be pumped away and modifies the polymer surface. The modifications of polymer on physical properties are investigated using conductivity, UV-vis spectroscopy, atomic-force microscopy (AFM) and confocal Raman spectroscopy. Hence, these all data provides new methodology for the modification of low bandgap polymer.

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Influence of Ammonium and Imidazolium Families Ionic Liquids on the Physical Properties of Polyaniline

김영범 차주현 김인태*

광운대학교 화학과

In this study, we investigate the effect of the two ionic liquid (IL) families such as ammonium and imidazolium families. Triethylammonium hydrogen phosphate (TEAP), Diethylammonium dihydrogen phosphate (DEAP), Tributylmethylammonium methyl sulfate (TBMS) are belongs to the ammonium IL family.While, 1-butyl-3-methyl imidazolium chloride ([Bmim]Cl) and 1-methylimidazolium chloride ([Mim]Cl) belongs to the imidazolium family ILs. We have observed that ILs has significant on the morphological, structural, and electronic properties of polyaniline (PANI). Physical properties of the PANI and IL combinations were characterised by SEM, UV-Vis, conductivity and Atomic force microscopy (AFM) measurements. The ILs addition strongly influenced the PANI morphology, specific surface area, and conductivity. Ammonium ILs modifies the physical properties of PANI more than imidazolium ILs.

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Writing behaviours of photoresponsive liquid crystalline elastomer

윤원진 최유진[1] 이명훈 정광운[2,*]

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A novel photoresponsive elastomer(PLCE) was synthesised via the acrylic diene metathesis polymerization. From the combined the techniques of DSC, POM and 2D WAXD, it was realized that PLCE formed a nematic (N) LC ordered phase containing the cynclinically tilted SmC-type cybotactic clusters, in which packing structure is related to the head-to-side connected PLCE chemical structure. Additionally, we demonstrated the rewritable micro-patterned PLCE film by using light and/or heat. Due to the wireless remote controllability of reversible actuating and patterning behaviors of PLCE. This work was mainly supported by the Converging Research Center Program (2013K000404), and BK21 PLUS Program, Korea.

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Phase transition of rod-disc by surface anchoring interaction

최유진 윤원진[1] 정광운[2,*]

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Rod-disc liquid crystal (LC) molecule (RD12) was newly designed and synthesized for characterizing and understanding of surface-induced phase transition behaviors of RD12 by changing the surface chemistry and the physical interactions. Upon varying the LC cells thickness and their surface chemical and physical environment, the RD12 phase transition behaviors were dramatically changed compared with in the bulk. The nematic phase of RD12 in the LC cell with a low cell gap and polyimide rubbed surface could be preserved and the crystallization of RD12 was thoroughly controlled. On the basis of the synthematic experimental investigations, it was realized that glassy N phase was formed because the interaction between surface alignment layer and RD12 is bigger than that of RD12 themselves This work was mainly supported by the Converging Research Center Program (2013K000404), and BK21 PLUS Program, Korea.

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5,5'-Di(heptadecan-9-yl)-4H,4'H-[1,1'-bithieno[3,4-c]pyrrole]-4,4',6,6'(5H,5'H)-tetraone-based Donor-Acceptor Alternating Copolymers containing Thiophene and Selenophene-based Monomers

이대희 박지은 엄현아 신지철 조민주 최동훈*

고려대학교 화학과

Recently, the D-A polymers based on thieno[3,4-c]pyrrole-4,6-dione (TPD) have received much attention due to its high performance in polymer solar cells and organic thin film transistors. TPD possesses a compact, symmetric, and planar structure, the strong electron-withdrawing imide group of TPD greatly lowers the HOMO and LUMO energy levels. In this study, we demonstrate the synthesis of new TPD-based copolymers containing thiophene and selenophene moieties as donor monomers. Thermal analysis, cyclic voltammetry and absorption spectroscopy were employed to investigate their physical and molecular electronic properties. Eventually, we fabricated electronic devices to study their p-type semiconducting properties.

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Synthesis and Semiconducting Properties of Diketopyrrolopyrrole-based Conjugated Polymers

양다슬 신지철 조민주 최동훈*

고려대학교 화학과

Diketopyrrolopyrrole (DPP) is an electron deficient dye with planar structure and forms intermolecular hydrogen bonds that result in materials with strong π-π stacking interactions. It has been studied a lot as a strong acceptor in a number of polymers. For more enhancement of charge transport properties, we synthesized a new diketopyrrolopyrrole based conjugated polymer containing siloxane side chains. It is already verified that a side chain with siloxane group has advantage in facile packing of polymer chains. For comparison, we also synthesized a known polymer with 2-decyltetradecyl side chains. Thermal analysis, absorption spectroscopy, and electrochemical analysis were employed to compare their properties. Eventually, we fabricated organic thin film transistors to study their semiconducting properties.

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Stability of Polymer Solar Cells with Ternary Bulk Heterojunction Layers

남성호 김화정 김영규*

경북대학교 화학공학과

Polymer solar cells (PSCs) with bulk heterojunction (BHJ) nanolayers have been extensively studied because of their prospect for low-cost flexible/lightweight solar modules that can be fabricated by utilizing continuous roll-to-roll processes at low temperatures. Recently the power conversion efficiency of PSCs has been significantly improved thanks to new low-band gap polymers and advanced fabrication technologies. However, the stability of PSCs is still remained as one of the significant issues toward commercialization. Recently we attempted to approach the stability (lifetime) issue by introducing ternary BHJ nanolayers. This presentation shows the performance of PSCs with the ternary BHJ nanolayers and then discusses on the lifetime improvement.

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Fused thiophene-containing Donor-acceptor Conjugated Polymers: Correlation between Structure of Donor Moiety and Charge Carrier Mobility for Organic thin film transistor

박지은 신지철 조민주 최동훈*

고려대학교 화학과

Recently, the most of high hole-mobility polymers are donor-acceptor (D-A) type materials including a strong electron-accepting and an electron-donating unit. Among these D-A copolymers diketopyrrolopyrrole (DPP)-based copolymers have gained much attention for their promising application in OFETs. Moreover fused-thiophene as donor unit containing polymer systems showed much higher charge carrier mobility due to strong strong stacking interaction in the solid state. In this study, we synthesized new low bandgap alternating conjugated copolymer containing tetrathienoacene (TTA) and dithienothiophene (DTT) which are fused heteroaromatic ring monomers and characterized their physical properties. Thermal analysis, cyclic voltammetry and absorption spectroscopy were also employed to investigate their unique properties. Finally, we fabricated thin film transistor devices to study their charge carrier transport properties.

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ZnO compact layer based perovskite solar cell

송슬기* 박태호*

포항공과대학교 화학공학과

Many researchers have tried to achieve flexible solar cells, organic light emitting diodes, flexible displays, e-paper, thin-film transistors and so on. Especially flexible solar cells are getting mass appeal. To achieve the flexible solar cells, however, many factors should be considered like stability, sealing problem, efficiency, processibility. Perovskite solid state solar cells are perfect device which could fulfill these requirements. Perovskite have been used in nanostructured solar cells as the sensitizer as well as hole transporter. It cna prepared in easy way. Besides, it showed efficient electron and hole transport ability. We employed the ITO/PEN/TiOx/Al2O3/spiro-OMeTAD use as a hole transporting material. Flexible solid state solar cell showed excellent stable efficiency when they bended. In this report, we assembled perovskite solar cells on the flexible substrate and it showed bright future of the flexible solar cells.

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Interfacial glass transition of thermoplastic filament extruded out of 3D printer nozzle

조애리 신관우[1,*] 권오선[*]

서강대학교 화학과 [1]서강대학교 화학과 및 바이오융합과정

Recently, 3D printing has been emerged as an attractive technology. It seems to promise opening a new era of the printing revolution following the pressing printing. In fact the gear of technical developing progress has been already changed up that it could lead the third industrial revolution. It is not a strange phenomenon because the 3D printing relies on the digital, desktop and additive manufacturing process and also being capable of complementing to the current subtract technologies in pressing and milling processes for manufacture. Among various methods, we here focused on studying the interfacial phase transition of the extruding thermoplastic filament emitted from the nozzle in a specific 3D printing type of Fused Deposition Modeling (FDM). Since we think that the most important physical and chemical parameter determining the shape of product is in the state of interfacial glass transition of filament. Here we represent the experimental concept for the contact angle on different surface conditions, high speed images of extruded filament and based on them analyzes the phase transition of thermoplastic filament especially on the hot base plate of printer. We conclude that the initial condensation of filament is most critical factor (Fig.1) to deposition of designed shape, layer by layer, and suggested the better modification for more stable and higher printing quality for FDM method.

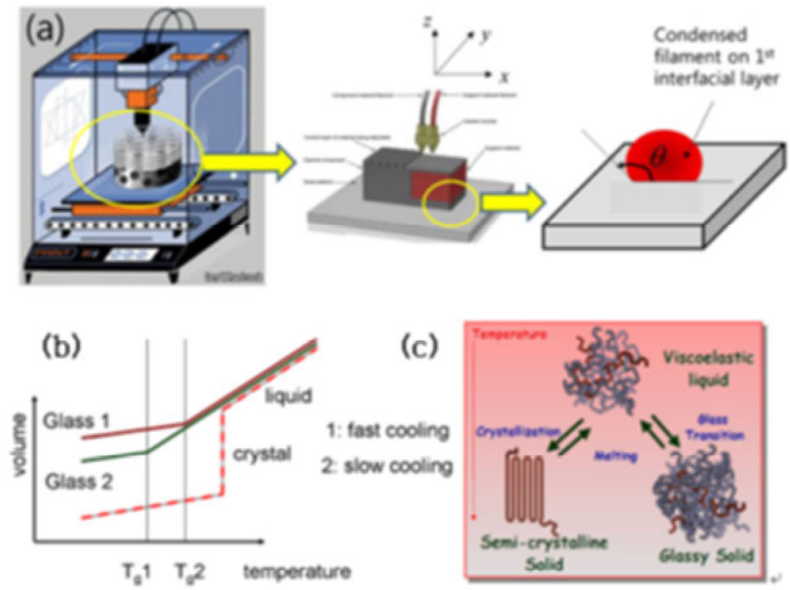

Fig. 1. (a) Schematic view of all of 3D printing processes. (b) Phase diagram of extruded thermoplastic filament, (c) Three phases of thermoplastic depending on temperature.

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Simple fabrication method of aligned doubly open-ended TiO2 nanotubes by a selective etching process, and their application in solar cells

최종민 박태호*

포항공과대학교 화학공학과

Anodic TiO_2 nanotubes (TNT) on Ti foil are most frequently employed as photoanodes due to high electron collection efficiency, but opacity of the Ti substrate, it requires back-side illuminations which decreased light harvesting. It is remained a challenge to produce TNT on transparent glass with good morphology for front-side illuminations. In this study, we describe a simple selective etching method to produce both open-ended TNTs membrane. The novel selective method employed the difference of chemical stabiltiy of double layers of TNT. Prepared aligned doubly open-ended TNTs that could be easily transferred to an FTO substrate for the fabrication of front-illuminated dye sensitized solar cells (DSCs). The TNT-DSCs yielded a higher PCE (8.6%) than was observed from TiO_2 nanoparticle-based DSCs (7.3%), for comparable film thicknesses of 16 micro meter, despite the use of 20% less dye. Intensity-modulated photocurrent and photovoltage spectroscopy revealed that the TNT-DSCs exhibited electron lifetimes that were 10 times longer than those of TNP-DSCs, which contributed to high device performances.

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Active hydrogen repulsive barrier comprised of polymer multi-layers

박민욱 박순천 정광운[1,*]

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The purpose of this study is to describe how the active hydrogen repulsion layer is constructed and works. The active hydrogen repulsion layer having excellent permeable resistance can be applied directly or indirectly to the hydrogen storage tank, semiconductor industry and gas barrier area. Active hydrogen repulsive barrier is successfully fabricated by multi-stacking polymer layer-by-layer layers, Nafion layer, platinum/palladium catalytic metal layer, and electrode layer on the poly(ethylene terephthalate) film. The most important point of the active repulsion layers is that the hydrogens are dissociated into the protons and electrons by electrochemical reactions. The generated protons are presented in the Nafion polymer electrolyte layer, on the other hand, the produced electrons are emitted through the electrode along the conductive wire.

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Modifiable Film Morphologies of Brush-Linear Diblock Copolymer Bearing Difluorene Moieties Yield a Variety of Digital Memory Properties

이호열 이문호* 고용기 김경태 김미희 김영용[1] 김종현 이진석 이종찬 김용진[1]

포항공과대학교 화학과 [1]포항공과대학교 첨단재료과학부

An amphiphilic brush-linear diblock copolymer bearing a rigid difluorene moiety was synthesized, yielding a copolymer with a high thermal stability and excellent process ability. The immiscibility of the blocks induced the formation of a variety of nanostructures, depending on the fabrication conditions, which differed significantly from the nanostructures observed among common diblock copolymers in similar composition. Interestingly, the orientations of the nanostructures could be controlled. The nanostructured polymer displayed a variety of tunable morphologies that yielded distinct electrical memory properties when incorporated as the active layer into a digital memory device. The memory devices could be operated under very low power consumption levels and displayed excellent unipolar switching properties.

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Synthesis and Characterization of Dithieno[3,2-b:2',3'-d]thiophene (DTT) Containing Conjugated Polymers

양훈주 안택*

경성대학교 화학과

Dithieno[3,2-b:2',3'-d]thiophene (DTT) has emerged as an important building block in the synthesis of a wide variety of optoelectronic materials. Thus DTT derivatives have been used in photo- and electroluminescent devices, two-photon absorption, non-linear optical chromophores, and photochromic materials. Here, we report the synthesis of two new DTT containing conjugated polymers such as poly(dithieno[3,2-b:2',3'-d]thiophenevinylene-alt-9,9-diethylhexyl-2,7-fluorenediylvinylene) (FLU-DTT) and poly(dithieno[3,2-b:2',3'-d]thiophenevinylene-alt-2-methoxy-5-(2-ethylhexyloxy)-p-phenylenevinylene) (MEH-DTT). The photoluminescence (PL) spectra of FLU-DTT and MEH-DDT showed the emission maxima at 528 and 578 nm, respectively as solution states. Interestingly, MEH-DDT showed far more red-shifted electroluminescene (EL) emission at about 650 nm. Detailed synthetic routes and light emitting properties of DTT containing conjugated polymers will be discussed.

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Reverse CO_2/N_2 selectivity membranes based on microporous organic molecular network/polyimide nanocomposite

전은경 박지웅[1,*]

광주과학기술원(GIST) 신소재공학과 [1]광주과학기술원(GIST) 신소재공학부

We synthesized microporous nanocomposites by controlling the interplay between phase separation and sol-gel transition in mixture of organic molecular networks(OMNs) and polyimide. The OMNs can generate nanochannels via thermal rearrangement of urea groups. The polyimide domains dispersed in the OMNs matrix provide dimensional stability against thermal deformation. Thin membranes of the OMNs/PI nanocomposites exhibit reverse selectivity: the observed CO_2/N_2 selectivity was about 0.15 in sharp contrast with that known in the conventional polymer membrane of 3~100.

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Synthesis and Photophysical Properties of Hyperbranched Conjugated Poly(para-phenylene vinylene) Derivatives

양훈주 이재민[1] 안택[*]

경성대학교 화학과 [1]한국화학연구원 소자재료연구센터

Conjugated polymers have emerged as viable electronic materials for numerous applications. So far, the majority of work on conjugated polymers has been focused on linear one-dimensional polymers. Although a few of two-dimensional conjugated polymers, such as hyperbranched conjugated polymer have been reported to exhibit comparable charge transferring and processing properties to their linear counterparts, two-dimensional conjugated polymeric light-emitting materials have been less discussed in the literature. Here, we report the synthesis and light-emitting properties of hyperbranched conjugated poly(para-phenylene vinylene) derivatives through A2 and B3 type monomer. A synthesized carbazole containing hyperbranched polymer showed pure blue emission as film state at 450 nm in photoluminescence (PL) measurement and was found to showing almost no excimer emission peak even the polymer film was annealed at 80 ℃. Detailed synthetic routes and photo physical properties of hyperbranched conjugated poly(para-phenylenevinylene) derivatives will be discussed.

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Selective molecular filtration membrane of ultrathin covalent organic networks by pore-limited molecular layer deposition

변민선 박지웅*

광주과학기술원(GIST) 신소재공학부

A new nanofilm composite (NFC) membrane is demonstrated. A solution-based, nanopore-limited molecular layer deposition (MLD) is conducted on a nanoporous alumina support to fabricate molecular nets as an ultrathin skin layer. Alternating deposition of multi-functional, tetrahedral molecules gives nanometer thick films of three-dimensionally cross-linked organic molecular networks. To achieve high-flux, high selectivity in filtration performance, it is essential to have ultrathin, net-like membranes with molecular level thickness. Varying the number of deposition cycles enables to control the pore size of the NFC membrane precisely on the molecular level. Molecular sieving performance confirmed by filtration of various aqueous solutions containing organic solutes. Molecular nets membrane is a promising strategy to overcome the limitations of the conventional separation system using membranes.

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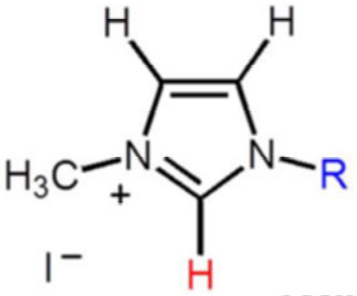
Highly Efficient Plastic Crystal Ionic Conductors for Solid-state Dye-sensitized Solar Cells

황대섭 김동영[1,*] 김동호[*]

연세대학교 화학과 [1]한국과학기술연구원(KIST) 물질구조제어연구단

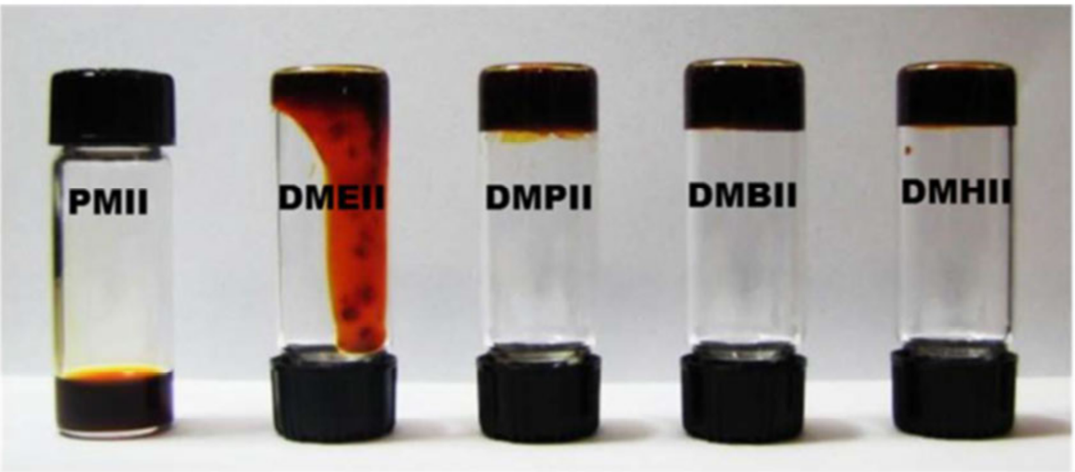
We have developed highly efficient, ambient temperature, solid-state ionic conductors (SSICs) for dye-sensitized solar cells (DSSCs) by doping a molecular plastic crystal, succinonitrile (SN), with trialkyl-substituted imidazolium iodide salts. High performance SSICs with enhanced ionic conductivity (2?4 mScm21) were obtained. High performance solid-state DSSCs with power conversion efficiency of 7.8% were fabricated using our SSICs combined with unique hierarchically nanostructured TiO2 sphere (TiO2-SP) photoelectrodes; these electrodes have significant macroporosity, which assists penetration of the solid electrolyte into the electrode. The performance of our solid-state DSSCs is, to the best of our knowledge, the highest reported thus far for cells using plastic crystal-based SSICs, and is comparable to that of the state-of-the-art DSSCs which use ionic liquid type electrolytes. This report provides a logical strategy for the development of efficient plastic crystal-based SSICs for DSSCs and other electrochemical devices.*Ref. : D. Hwang et al., Nature Sci. Rep., 3, 3520

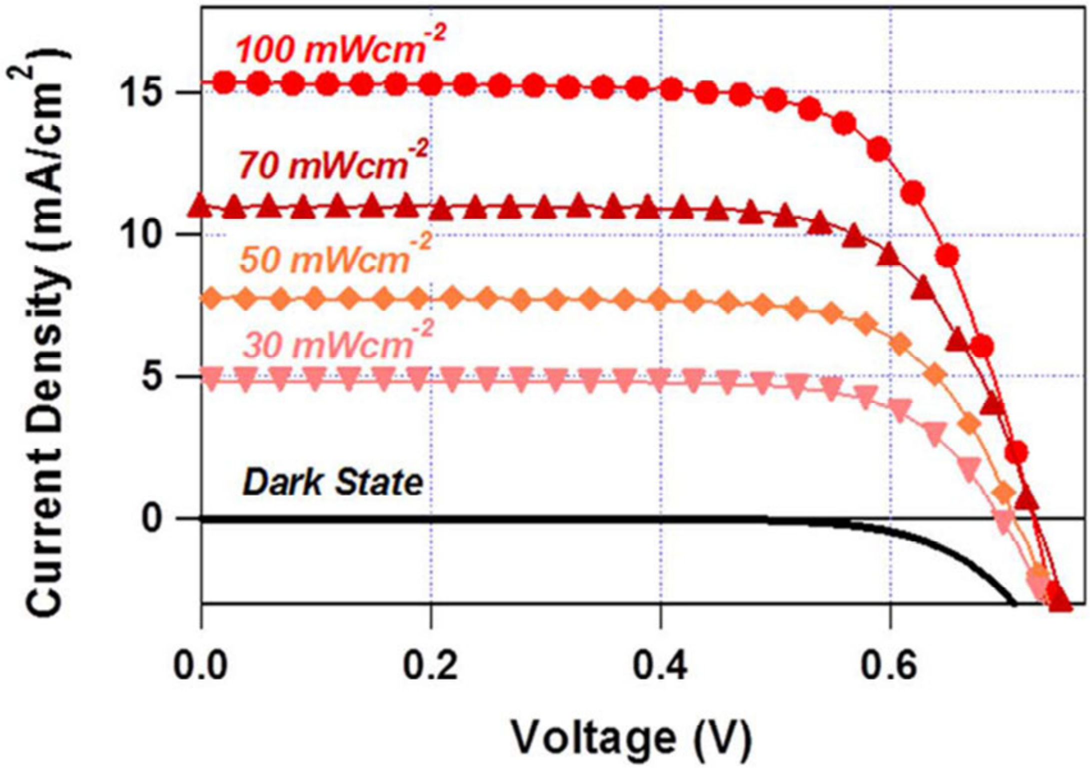


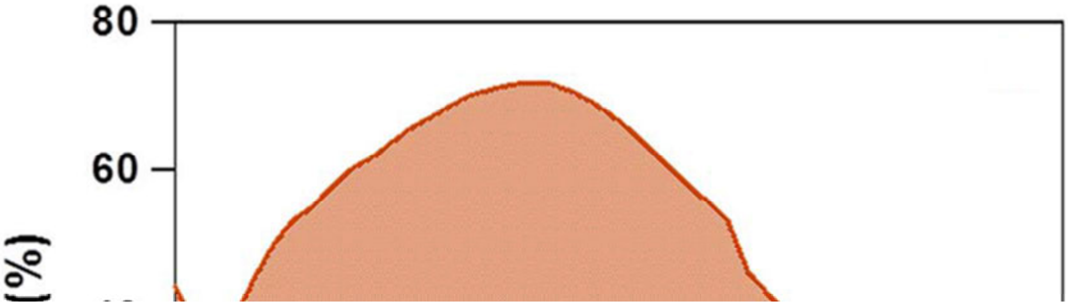
AMII

DMAII

R= ethyl (DMEII)
propyl (DMPII)
butyl (DMBII)
hexyl (DMHII)





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발표종류: 포스터, 발표일시: 수 16:00~19:00

Low bandgap polymers containing a thienothiophene segment for organic photovoltaic devices

김홍기 이윤구[1,*]

대구경북과학기술원(DGIST) 에너지시스템공학 [1]대구경북과학기술원(DGIST) 에너지시스템공학전공

Organic photovoltaic devices (OPVs) have attracted considerable attention because of their advantage of light weight, flexibility, and low costs of materials. So far, a power conversion efficiency of ~5% has been obtained in OPVs using P3HT and PCBM. To achieve high power conversion efficiency (PCE) in OPVs, it is necessary to develop new p-type polymers which possess several characteristics such as harvesting photons in a wide range of spectrum, efficient exciton dissociation, high hole mobility, suitable HOMO and LUMO energy levels, and good miscibility with the electron-acceptor materials. In this work, we successfully synthesized a variety of p-type polymers containing a thieno[3,4-b]thiophene segment for OPVs. The polymers exhibited low bandgap characteristics because the thieno[3,4-b]thiophene segment can induce a quinoidal structure inside a polymer backbone. The device performances of bulk heterojunction OPVs with new p-type polymers will be presented.

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Synthesis and characterization of cationic water soluble conjugated polymer

남궁한솔 박동규*

경성대학교 화학과

We have synthesized cationic water soluble conjugated polymer, Poly[1,1'-((2-methyl-7-(7-methylbenzo[c][1,2,5]thiadiazol-4-yl)-9H-fluorene-9,9-diyl)bis(hexane-6,1-diyl))bis(pyridin-1-ium) bromide](PMMBTD-FHPB), as the role of electron transport materals. The polymer typically obtained by the Suzuki type of polymerization reaction and shows good solubility in methanol. The band gap energy of the polymer was estimated from the absorption spectrum and was found to be 492nm (2.52 eV).

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Crosslinkable sPPO composite membrane by LbL for DMFC applications

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한양대학교 유기나노공학과

Layer-by-layer (LbL) deposition is a very versatile method to prepare very thin polyelectrolyte multilayer composite films. LbL method is often used for the surface property modification of a given polymer film. Here, we prepared multilayered composite PEM by LbL method on the surface of Nafion212. The sulfonated polymer mixture contains highly sulfonated poly(phenylene oxide) (sPPO) and polystyrene copolymer containing azide moiety. Crosslinked composite membrane was prepared by photochemical crosslinking using UV. The composition ratios of polymer layers were identified using H-NMR and FTIR. Also the layer thickness was shown to increase with the concentration of NaCl in the bath. Although the proton conductivity was slightly lower than that of Nafion, a 40% reduction of methanol permeability ultimately leads to an increased overall selectivity. This proves that the UV crosslinking method can be applied to other LbL composite films as well as flat fuel cell membranes.

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Polyelectrolyte Multilayer Films Composed of Multistimuli-Responsive Diblock Copolymer Micelles

김순화 빈센트 홍종달*

인천대학교 화학과

Stimuli-responsive polymer films that control adhesion, wetting, and binding or release of functional molecules from surfaces are promising candidates for drug delivery, sensing, and tissue engineering applications. The property of stimuli-responsive polymers changes dramatically in response to external conditions. Among the interesting features of responsive polymers is their reversible micellization in solution in response to external stimuli, e.g. changes in temperature or pH.Herein, we report on assembly and stimuli-response behavior of temperature- and light responsive diblock copolymer micelles of newly-designed poly[N-isopropylacrylamide-block-vinylmalachite green] (PNM), which was synthesized by reversible addition fragmentation transfer (RAFT). The copolymer PNM has thermo-responsive block N-isopropylacrylamide and a light-responsive block malachite green. The malachite green group is an electrically neutral hydrophobic group, which, however, can be ionized into its corresponding delocalized triphenylmethyl cation upon UV irradiation. The transitions of PNM unimers to conventional micelles relying on solution temperature, UV irradiation and pH were studied. The multi-responsive block copolymer PNM was LBL deposited onto a solid substrate or a nanoporous alumina membrane using electrostatic self-assembly technique. The influence of the aggregate size of the PNM block copolymer in aqueous solution on the quantity and thickness of the multilayer films layer-by-layer (LBL) assembled with poly(acylic acid) PAA on a solid substrate is being investigated as a function of solution temperature and light-exposure length using UV/visible spectroscopy, optical ellipsometry, and AFM. The ion transport through the PSN membrane will be reversibly controlled in response to the thermal, pH, and light stimuli for the development of “smart” functional materials, which could be applied in various fields, such as biotechnology, drug delivery, particle transport, and optical sensing.

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Characteristic evaluation of hydroxyapatite-PLA scaffold using modified solvent/non-solvent sintering and centrifugation methods

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The previous study, the scaffolds were fabricated by the solvent and non-solvent sintering and centrifugation method using poly(D,L-latic-co-glycolic acid)(PLGA) porous microparticles and hydroxyapatite(HA) which was known to help for cell movement, proliferation and differentiation of bone and cartilage. It was found that they had the low physical property and fast degradation rate. In this study, Poly(lactic acid)(PLA) was used as a scaffold material instead of PLGA, because scaffolds for bone tissue need to have the enough mechanical properties. Shape, porosity and chemical compositions of PLA scaffold were shown to be different from PLGA scaffolds. Moreover, higher mechanical properties could be observed. Therefore PLA-HA scaffold seems to be a potential material for bone tissue engineering.

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Edge-functionalized graphene nanoplatelets with iodine/SO3 via ball milling

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We have prepared edge-iodine/sulfonic acid-functionalized, graphene nano-platelets (ISGnP) via two-step sequential ball-milling of graphite, and their use as electro-catalyst for oxygen reduction reaction (ORR) in fuel cells. The graphite is ball-milled in the presence of iodine to produce edge-iodine functionalized GnP (IGnP) in the first step and the IGnP is subsequently ball-milled with sulfur trioxide to yield ISGnP. The resultant ISGnP is highly dispersible in various polar solvents, allowing the fabrication of electrodes for ORR using solution processing. The ORR performance of ISGnP in an alkaline medium is superior to commercial Pt/C in terms of electro-catalytic activity and cycle stability.

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Small angle neutron scattering study of temperature and time dependent polymer behavior

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Poly(2-((3-(1-(2-(dimethylamino)ethyl)-1H-1,2,3-triazol-4-yl)propanoyl)oxy)ethyl methacrylate), P1, which has great attention due to a lot of applications for biochemistry and bio-engineering, was prepared and characterized depending on temperature, pH and time. P1 solution properties were probed with small angle neutron scattering (SANS) and dynamic light scattering (DLS). P1 exhibited cloudy phase transition above a certain temperature and the cloud point depended on the incubation time in solution at room temperature. SANS and DLS studies showed that P1 formed clusters by hydrophobic effect and weakened hydrophobic effect by polymer dissolution with incubation time consequently attributed to decrease in size or disappearance of clusters. The temperature dependence of cluster formation can be explained by hydrophobic effect with both the increase in scattering intensity by clusters at low q region and the decrease in correlation length of polymer at high q region based on 'two Lorentz model' analysis. Decreasing intensity of clusters on the scattering patterns of P1 with increasing incubation time shows weak cluster formation. Decrease of Porod exponent of P1 solution below cloud point reflects the dissolution change of P1 from mass fractal of branched polymer to loosen structure of polymer chains as incubation time increases.

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Synthesis of Glucose-Responsive Self Assembled Multilayer Films and Their Application in Controlled Drug Delivery

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인천대학교 화학과

Phenylboronic acid (PBA) polymers are important precursors to materials with potential utility in catalysis, separations, and sensing applications. These water soluble polymers are known to form complexes with polyol compounds such as glucose and have demonstrated promise in biological applications as well, having gained a great deal of attention for glucose or RNA sensing, diabetes treatment therapies, and as supramolecular materials. Herein, we report the synthesis of novel copolymers containing PBA as a glucose sensing moiety and malachite green (PBA-*co*-PMG) or spiropyran (PBA-*co*-PSP) as the photo-responsive moiety by free radical polymerization. The solution self-assembly of these multistimuli-responsive copolymer unimers to micelles in response to the changes in sugar concentration, optical and pH stimuli were studied. The copolymers were layer-by-layer deposited onto a solid substrate along with a positive charged polyelectrolyte using electrostatic self-assembly technique. The morphology change of the multilayer films, which respond to glucose concentration, optical, and pH stimuli are investigated using UV/visible spectroscopy, optical ellipsometry, and AFM. Moreover we report the controlled release of the fluorescent labeled insulin loaded into the multilayer films in response to glucose concentration and pH, for the development of smart materials which held’s great potential in biotechnology, drug delivery and optical sensing applications.

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Efficient Organic dye composed of Triphenylamine Chromophore for Dye-sensitized Solar Cells

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영남대학교 화학공학부

Organic dyes are suitable as photosensitizers for the Dye-sensitized Solar Cell (DSSC) because they have many advantages, such as high molar extinction coefficients, convenience of customized molecular design for desired photophysical and photochemical properties, inexpensiveness with no transition metals contained, and environment-friendliness. Generally, people know that the efficiency of DSSC based on metal-free organic dyes is much lower than that of Ru dyes, but a high solar energy-to-electricity conversion efficiency of up to 8% in full sunlight has been achieved by Ito et al using an indoline dye. This result suggests that smartly designed and synthesized metal-free organic dyes are also highly competitive candidates for photosensitizers of DSSCs with their advantages mentioned above. Organic photosensitizers based on triphenylamine with multi-acceptors/anchors chromophores were synthesized and applied to DSSCs.The judicious choice/design of the donor and acceptors permits the relatively high power conversion efficiency of 4.7 % (TPA3TCN) in organic dye containing cyanoacrylic acid as the electron acceptor

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F?rst Resonance Energy Transfer(FRET) System Energy Acceptors and Donors for the Quasi-solid State of Dye-sensitized Solar Cell

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영남대학교 화학공학부

Various energy transfer processes have attracted extensive interest in biology and supramolecular chemistry. The F?rst-type resonance energy transfer (FRET) has been investigated to enhance the photovoltaic performance of solar concentrators or dye-sensitized Solar Cells (DSSCs). The fluorescence materials could absorb high-energy photons and transfer their energy to the sensitizing dyes via FRET process in DSSCs. Thus, the injection of electrons from the sensitizing dyes into the conduction band of photoelectrode could be enhanced by the energy transfer from the fluorescence material. Several kinds of F?rst type of resonance energy transfer were reported to improve the photovoltaic performance of sensitizers and the theoretical calculation for the FRET efficiency and their dynamics have been performed and verified for various energy donors and acceptors in DSSCs. In this paper, we added organic fluorescence materials on the photoelectrode and/or quasi-solid state electrolyte in order to increase the light harvesting performance of photosensitizer. The structure of the fluorescence materials was chosen carefully to emit the fluorescence that should be absorbed in sensitizers effectively to enhance photovoltaic performance of DSSCs.

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Highly efficient photovoltaic performance of quasi-solid-state dye-sensitized solar cells composed of the blended polymer electrolytes

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영남대학교 화학공학부

There has been an increasing interest in the dye-sensitized solar cells (DSSCs) owing to a potential for highly efficient solar energy-to-electricity conversion efficiency, low-cost and easy manufacturing process. From dye to electrolyte, there are various parts of DSSCs. This covers, inter alia, electrolyte issues in DSSCs. It is well known that the presence of traditional liquid electrolytes in dye-sensitized solar cells is related to problems such as precipitation of salts in the electrolyte at low temperature, evaporation of liquids of the electrolyte at high temperature, corrosion and lack of long-term stability of the cells. In order to overcome various problems associated with liquid electrolytes, quasi solid-state polymer electrolytes which is well known PVDF-HFP can be used in dye-sensitized solar cells.In this study, DSSCs based on quasi-solid type of electrolytes composed of Poly (vinylidene fluoride-co-hexafluoro propylene) and polymer were executed and the photovoltaic characteristics were summarized.The photovoltaic performances of the DSSCs composed of different polymeric materials of quasi-solid electrolyte compared using I-V curves, incident photon-to-current (IPCE) efficiencies, and impedance analysis to investigate the conducting properties of electrolyte.

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Hybrid Nanocomposites of Pd Nanoparticles and Poly(acrylic acid)-Grafted MWNTs with POSS through In-situ method

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한국교통대학교 나노고분자공학과

Multiwalled carbon nanotubes(MWNTs) have the excellent mechanical, electrical, thermal, and optical properties. Palladium nanoparticles with POSS (Pd-POSS) are good candidate for chemical, optical, magnetic, and electronic devices with useful properties. Organic-inorganic hybrid nanocomposites have high performances regarding the thermal stability, mechanical property, high gas barrier, flame resistance, transparency, and excellent solvent resistance property. In this study, we have prepared the composite of poly(acrylic acid)-grafted MWNTs (PAA-MWNTs) and POSS-NH3+ (MWNT-POSS) through the ionic interaction between positively charged POSS-NH3+ and negatively charged PAA-MWNTs. POSS-NH3+ was physically attached to the surfaces of PAA-MWNTs to make MWNT-POSS. MWNT/Pd-POSS was produced from the reaction of MWNT-POSS and palladium(Ⅱ) acetate in methanol at room temperature. The characteristics of the hybrid nanocomposites (MWNT/Pd-POSS) were characterized by various analytical tools.

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Cellulose-Based, Conjugated Polymer Composite Papers for the Detection and Removal of Metal Ions

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Here, we propose polypyrrole/cellulose (PPCL) composite papers as the efficient tool for the real-time detection and removal of metal ions in solution. We obtained PPCL papers via vapor deposition polymerization. The cellulose provided appropriate mechanical strength as the support while the polypyrrole afforded good electrochemical properties. The PPCL papers demonstrated the ability to discriminate electrochemically between metal ions in both static and flow cells. The PPCL papers when exposed to metal ions gave different profiles in response. The sorption of metal ions by the PPCL papers was examined in the flow system. The PPCL showed the best adsorption efficiency for Hg(II) between that of the other metal ions. These results demonstrate the strong promise of PPCL papers for development to flexible or wearable device of amperometric metal ion sensors with selective recognition and in situ uptake functions.

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The Effect of Substrate Curvature On The Morphology of Deposited Polymer Nanomaterials

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We describe the concept that the morphology of deposited polymer nanomaterials is subject to substrate curvature, as well as synthetic conditions. Nanonodules and nanorods can be grown on a nano?ber surface by controlling critical kinetic factors such as temperature and pressure during vapor deposition polymerization, leading to the formation of multidimensional polymer nanostructures. On the other hand, no remarkable nanostructures were generated on bulk ?at substrate under the same conditions. Multidimensional poly(3,4-ethylenedioxythiophene) (PEDOT) nano?bers were fabricated successfully, and their hollow nanostructures, namely nanotubes, were also obtained by a core-etching process. It is highly anticipated that the multidimensional polymer nanomaterials will have advantages when used as structures for filtration, separation, sensing, and energy conversion/storage.

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Solution-Processable Conductive Polymer Binders for Electrochemical Capacitors

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Developing new polymer binders for electrode materials is of considerable importance. Here, we report the preparation of an intrinsically conductive quaternary polymer binder through the combination of polyaniline (PANI) with three additives. The three additives acted as a ternary dopant for conducting and gluing properties of PANI, and thus the resulting PANI could have excellent conductivity and adhesive properties without the use of additional conductive fillers or heat-treatment processes. Importantly, the PANI binder itself had a high specific capacitance and therefore significantly improved the performance of capacitor electrodes when used as a binder. It is anticipated that our PANI binder will be suitable as an adhesive for emerging all-organic flexible or wearable devices.

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p-NIPAAm based thermo responsive copolymer with imidazolium moiety

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A series of stimuli-responsive copolymers (p-NIBIm) of N-isopropylacrylamide (NIPAAm) and 1-butyl-3-vinyl imidazolium bromide (BVIm) with various BVIm concentrations of 5 to 20 were synthesized by radical copolymerization. The concentration of imidazolium moieties within the resulted ionic copolymer chains was determined by ^{1}H-NMR and FT-IR analysis. The LCSTs (lower critical solution temperatures) of the copolymers were checked by DSC and they were ranged from 32 to 45 ^{o}C. The p-NIBIm copolymers showed increasing Zeta potential values (from +0.3 to +21.3 mV) and micelle size (about 175 nm ~ 325 nm). These results revealed that the thermo sensitive and ionic co-polymers have potential to be useful as a drug delivery system such as hypothermia or anticancer drug delivery system.

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Understanding the Mechanical Behavior of Patterned Polymer Sheets

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Understanding the mechanical behavior of patterned polymeric materials at large deformation is examined with respect to the diverse polar angle. The tensile force fluctuates as an undamped negative sinusoidal wave with a periodicity of 15°. The amplitude of the fluctuation is proportional to the thickness of the patterned polymer sheets, but the Young's modulus is independent of the thickness and the polar angle. Total and local Poisson's ratios of patterned polymer sheets at the 30° polar angle are lower than those obtained at the 0° polar angle over the entire strain range, and the difference becomes smaller. The experimentally observed structure-property relationship of the patterned polymer sheets can provide important signs for understanding the deformation behavior of patterned polymeric materials.

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Phosphoryltion of chitosan as a wound healing dressing accelerates the blood clot

<u>왕윤선</u>

한국과학기술원(KAIST) 화학과

Chitosan, the second most abundant polysaccharide, has been studied as biomedical material due to its biodegradability and biocompatibility. It is widely used as a wound healing dressing because it has a hemostatic potential. Herein we reported that phosphorylation of chitosan improved its hemostatic ability preserving the biocompatibility. Phosphorylated chitosan synthesized with a phosphorus pentoxide/ methanesulfonic acid system was confirmed by XRD, FT-IR, ^{31}P NMR, ^{13}C NMR, SEM. We tested the antibleeding properties of the modified chitosans with various ratio of phosphate substitution by applying them on a mouse hemorrhage liver. As a result, the modified chitosan with higher degree of phosphate reduced a blood coagulation time. The phosphorylation resulted in the porous and anionic surface of chitosan, which had important role in assembling proteins responsible for the blood clotting initiation. It indicated that phosphorylation accelerated the blood clot formation.

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New Small-molecule Donors based on DPP for OPVs

김유정 임은희*

경기대학교 화학과

Organic photovoltaic cells (OPVs) have received much attention as highly promising devices producing infinite, renewable and clean energy from sunlight. Recently, the highest PCE of 12.0% has been reported at Heliatek. In the past decade, bulk heterojunction solar cells based on conjugated donor materials have dominated in research because they have excellent film-forming characteristics and good film morphology, resulting in high efficiency of these cells. However, polymeric donors are associated with a number of difficulties owing to their poor synthetic reproducibility, difficult purification procedures, end-group contamination and broad molecular weight. In contrast to polymers, small-molecule materials have shown advantages over polymeric materials, which include easy synthesis, purification and functionalization. Among various factors for PCE such as Jsc, Voc and FF, Jsc could be increased by low band gap attaching electron-rich unit like thiophene next to core of donor. However, effort of making low Eg could elevate HOMO energy level with the result of decreased Voc. The other way, donors substituted with electron-withdrawing unit such as fluorine, cyano and carbonyl group could enhance Voc due to relatively low HOMO level but that also makes wide Eg. In this work, π-conjugated small molecules based on diketopyrrolopyrrole (DPP) core were synthesized containing electron-withdrawing unit to analyze substituent effect. The effect of substitution pattern and device optimization also will be presented.

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The physical prorerties of hydrogel ophthalmic polymer containing hydroxypyridine

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The high functional contact lens using 3-,4-hydroxypyridine as additives were manufactured and also the physical properties of the produced hydrogel lens were measured. This study used 3-hydroxypyridine and 4-hydroxypyridine as additions with the cross-linker, EGDMA (ethylene glycol dimethacrylate), HEMA (2-hydroxyethyl methacrylate), MMA (methyl methacrylate), AA (Acylic acid) and the initiator AIBN (azobisisobutyronitrile) for thermal copolymerization. The mixture was heated at 115 ℃ for 50 mins to produce the hydrogel ophthalmic lens. The polymer by using thermal polymerization process for hydrogel contact lens was copolymerized and the physical properties which showed that the contact angle of sample containing 3-hydroxypyridine and 4-hyroxy pyridine was in the range of 49.34~58.47° and 58.39~63.22°, respectively. The wettability of samples increased as the ratio of 3-,4-hyroxypyridine increased. Also in case of 3-hydroxypyridine showed that visible light 87.0~87.2%, UV-B 7.2~1.2%, UV-A 34.6~21.4% and in case of 4-hydroxypyridine showed that visible light 90%, UV-B 80.2~79.6%, UV-A 85.8~85.2%. The produced copolymer is suitable for hydrogel soft ophtalmic lenses with UV-blocking effect and high wettability.

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Characterization of hydrogel tinted ophthalmic lens containing 4-iodoaniline using Ag nanoparticles as additive

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The physical and optical characteristics of hydrophilic tinted ophthalmic lens containing Ag nanoparticles and 4-iodoaniline were examined. In this study, the utility of Ag nanoparticles and 4-iodoaniline as antimicrobial and UV-blocking materials for ophthalmologic devices were investigated by measuring the physical properties of the produced polymer.For manufacturing hydrogel lens, HEMA, MA, MMA, 4-iodoaniline and a cross-linker EGDMA were copolymerized in the presence of AIBN as an initiator. Also, the Ag nanoparticles was used as additive. After polymerization, the physical properties such as water content, refractive index, contact angle and spectral transmittance of produced ophthalmic lenses were measured. The results of the measurement showed that the water content, refractive index, contan angle and spectral transmittance of the hydrogel lens polymer was 37.63~ 34.28%, 1.4366 ~ 1.4450, 39.16 ~ 65.34° and 1.8 ~ 86.2%, respectively. Also, the transmittance for UV light was reduced significantly in mixture combinations containing 4-iodoaniline. The produced ophthalmic polymer material is expected to be used usefully as a material for fabricating UV-block hydrogel ophthalmic lens.

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Adsortive removal of 2,4-dichlorophenoxyactic acid (2,4-D) from water with Cr-benzenedicarboxylate metal-organic framework

정범근 정성화*

경북대학교 화학과

Removal of 2,4-dichlorophenoxyacetic acid (2,4-D) using a MOF (metal-organic framework), Cr-benzenedicarboxylate (MIL-53), has been studied for the first time to understand the applicability of MOFs in the adsorptive removal of hazardous herbicides from contaminated water. MIL-53 has a very fast adsorption in one hour and the adsorption capacity of MIL-53 is much higher than that of activated carbon or zeolite (USY). Importantly, the adsorption of 2,4-D over MIL-53 is very favorable especially at low concentrations of 2,4-D. Moreover, the adsorbent can be used several times in adsorptive removal by washing the used adsorbent with a simple solvent. Therefore, MOFs such as MIL-53 can be one of adsorbents that could be used in the adsorptive removal of 2,4-D from contaminated water. Additionally, zeta potential of the adsorbent and the effect of pH and temperature on the adsorption were also investigated, and a plausible adsorption mechanism could be suggested.Reference[1] B.K. Jung, Z. Hasan, S.H. Jhung, Chem. Eng. J. 2013, 234, 99-105

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Catalytic dehydration of bioalcohols with ZSM-5 zeolitic materials synthesized from hexamethylene imine and microwave ageing

전종원 정성화*

경북대학교 화학과

Hexamethylene imine (HMI) has been utilized as a template material to synthesize ZSM-5 zeolite. Microwave aging played very crucial role for the crystallization of ZSM-5 from gels. Moreover, adequate reaction conditions (such as Al2O3/SiO2, HMI/SiO2 and H2O/SiO2 ratios, pH, reaction time and so on) for ZSM-5 syntheses are also suggested. The obtained ZSM-5, after ion exchange to the proton form, can be applied in acid-catalyzed reactions because the acidity and surface area of the zeolite are very similar to those of commercial ZSM-5 zeolite. For example, the H-ZSM-5 can be applied in the dehydration of bioalcohols such as ethanol and n-butanol into olefins or aromatics, very similar to a commercial H-ZSM-5 zeolite.Reference[1] R. Barthos, A. Sz?chenyi, F. Solymosi, J. Phys. Chem. B 2006, 110, 21816?21825

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Adsorptive desulfurization with ionic liquid-supported metal-organic framework (MOF)

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경북대학교 화학과

Ionic liquid (IL)-supported metal-organic framework (MOF) was firstly demonstrated for the beneficial utilization of acidic IL in adsorptive desulfurization [1]. For that, 1-butyl-3-methylimidazolium chloride (a typical IL) was introduced to one of the widely studied MOFs, MIL-101 (chromium-benzenedicarboxylate) [2] via simple impregnation at ambient condition. A remarkable improvement in the adsorption capacity (~71%) was observed in IL-supported porous MIL-101 compared to the virgin MIL-101 for the adsorption of benzothiophene (BT) from liquid fuel. The improved adsorptive performance could be explained by the acid-base interactions between the acidic ionic liquid and basic BT. Moreover, from this study, it can be suggested that porous MOFs, supported with ionic liquids, may introduce a new class of highly porous adsorbents having the advantage of the imidazolium cationic sites for the efficient adsorption of various compounds.References[1] N.A. Khan, Z. Hasan, S.H. Jhung, Chem. Eur. J. 2014, 20, 376-380. [2] G. F?rey, C. Mellot-Draznieks, C. Serre, F. Millange, J. Dutour, S. Surble, I. Mirgiolaki, Science 2005, 309, 2040-2042.

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초기 유기 박막 성장 동안 보이는 분자 배향에 규칙성의 질서-무질서 전이

배우리 김진형[1] 조양진[2] 강상욱[2,*]

고려대학교 세종캠퍼스 일반대학원 소재화학과 [1]호서대학교 광전자디스플레이공학 [2]고려대학교 소재화학과

photoelectron spectroscopy (PES)을 사용하여 매우 규칙적으로 정렬 된 열분해 흑연 (HOPG)의 표면에서 1,3-bis(N-carbazolyl)benzene (mCP) 박막 필름의 최초로 성장하는 동안 분자 배향 식별과 규칙성의 질서-무질서 전이 식별에 관하여 연구를 진행하였다. independent atomic center approximation (IAC)을 적용하여 양자 역학적으로 계산한 이론상의 PES 진폭은 실험적인 관측과 비교하기 위하여 계산 하였다. 이 방법은 분자 방향의 체계적인 추정과 특이한 구조의 분자에 대한 규칙성의 무질서를 제공한다. 낮은 범위에서, 절연된 흡착의 평형 방향이 추정되었다. 그러나, 적용 범위가 증가함에 따라 각 피크의 라인 폭 증가뿐만 아니라 PES 구조의 변화의 결과로써 흡착물 사이의 상호작용이 지배적으로 되고 규칙성의 무질서가 증가하였다.

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Carborane 에서 보이는 새로운 광 동역학적 Multiple Photoluminescence 연구

조양진 김소연[1] 강상욱*

고려대학교 소재화학과 [1]고려대학교 세종캠퍼스 소재화학과

Decarborane 과 Naphthyl 기가 치환된 acetylene 의 합성을 통해 ortho-carborane 의 탄소의치에 1, 2 번 위치의 Naphthyl 기가 치환된 화합물을 합성하였다. 합성된 화합물을 여기시켰을 경우 Naphthyl 기 고유의 발광(380 nm) 및 인접한 Naphthyl 기에 의한 excimer 발광(420 nm), Naphthyl 기와 ortho-carborane 분자내 전하이동에 의한 발광(510 nm, CT emission) 이 섞인 multiple photoluminescence 가 관측 되었다. DFT 계산결과를 토대로 ortho carborane 에서 보이는 특징적인 CT emission 은 Naphthyl 기의 π-orbital 과 ortho-carborane 의 σ*-orbital 의 중첩에 의해 이러한 상호작용에 의해 photoluminescence 가 발생함을 확인 하였다. 또한 Naphthyl 기의 2 번 위치가 치환된 화합물의 경우, 치환체의 운동이 구조적으로 제한되어 orbitl 의 중첩이 1 번 위치가 치환된 화합물보다 더 큰 것을 알 수 있었다.

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다공성 실리카 채널을 이용한 AB 수소발생에서 금속의 담지

원동일 지정민[1] 강상욱[1,*]

고려대학교 소재화학 [1]고려대학교 소재화학과

테트라글라임(tetraethylene glycol dimethyl ether;TG) 용매상에서 SBA-15(Santa Barbara Amorphous-15)이라는 실리카 채널로 팔라듐나노입자(Palladium nanoparticles;PdNPs)를 담지하였다. 우선적으로 전자 단층촬영(Electron tomography)과 고분해능 전자투과현미경(HRTEM)을 통해 PdNPs 가 실리카 채널 속에서 평균 8nm 의 지름으로 균일하게 형성되는 것을 확인하였다. 또한 이 방법을 Au, Ag 에 적용시켜 크기 조절이 가능한 금나노입자와 은나노입자가 형성되는 것을 확인하였다. 이 반응 방법은 매우 간단하고 재생산이 가능하며, 전처리 과정이 없다. 생성된 PdNPs/SBA-15 을 이용하여 암모니아보란(NH_3BH_3;Ammonia borane)의 수소발생 속도를 향상시켰다. PdNPs/SBA-15 은 PdNPs 와 비교하여 매우 큰 TON(turnover numbers)을 보였으며, PdNPs/SBA-15 의 TOF(turnover frequency)는 9760h^{-1} 로 PdNPs 와 비교하여 10.4 배 높았다. 암모니아 보란의 수소발생에서 PdNPs/SBA-15 의 중요한 장점은 촉매 회수를 통한 재사용이 가능한 것이다.

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이리듐 기반의 dendrimer에서 보이는 페닐카바졸 단위체에서의 light-harvesting 연구

오태훈 장설[1] 조양진[2] 강상욱[2,*]

고려대학교 세종캠퍼스 소재화학 [1]고려대학교 세종캠퍼스 에너지미래연구소 [2]고려대학교 소재화학과

높은 인광 발광을 나타내는 이리듐을 중심금속으로하고 카바졸을 dendron 으로한 dendrimer 에서 에너지 전달 메커니즘을 통한 인광효율 증가를 측정했다. 이리듐 core/페닐카바졸 형태 $Ir(dfppy)_2(pic\text{-}Cz_n)$ (Gn, n = 0, 1, 2, and 3)에 카바졸 단위체 치환을 통한 카바졸 단위체 증가로 선택적인 들뜬 상태를 보였다. 그로 인한 연속적인 에너지 전달로 90% 이상의 형광 에너지 감소와 인광 에너지 증가를 보였다. 에너지전이 반응속도가 4.32 $*10^9$ s^{-1} (G1), 2.37 $*10^9$ s^{-1} (G2), and 1.46 $*10^9$ s^{-1} (G3) 와 같이 감소하는 것을 Fo¨rster model 를 이용하여 계산하였다. $Ir(dfppy)_2(pic\text{-}Ph_2)$코어를 사용한 G0 와 비교 했을 때 인광효과 증가는 G1-157%, G2-214%, G3-264% 와 같이 나타났다.

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새로운 염료-TiO_2-Re구조 에서 보이는 높은 광전환 효율의 CO_2 환원 연구

원동일 지정민[1] 조양진[1] 강상욱[1,*]

고려대학교 소재화학 [1]고려대학교 소재화학과

가시광을 이용하여 CO_2 환원을 시키기 위해 TiO_2 반도체에 흡광체로 유기염료 (DMOM)와 CO_2 환원촉매로 Re(I) complex 를 접합시킨 구조를 제시하였다. 광전환 시스템에서 전자주개(SD)로는 SDN 을 사용 하였다. 가시광 영역인 420 nm 빛을 광조사 하였을 경우 DMOM 이 광자를 흡수하여 들뜬 전자를 TiO_2 의 conduction band 로 넘겨주고 이 전자는 Re(I)촉매로 이동하여 CO_2 가 CO 로 전환되는 메커니즘을 제시 하였다. 이때 전자를 건네 준 염료는 SDN 에 의해 전자를 제공받아 재생되는 구조를 이루고 있다. TiO_2 는 3 그룹으로 나뉘어 실험이 진행되었으며 결정형의 [001] facet (S-TiO_2)와 분말형태의 Hombikat UV-10 (H-TiO_2), Degussa P-25 (D-TiO_2)를 이용하였으며 H-TiO_2 를 사용하였을 때 가장 높은 광전환 효율을 보였다. 최적화된 구조에서 1600 min 동안 광전환 실험 결과 TN(turnover number) = 435 를 보였다.

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고정된 구조의 세개의 Phenyl기가 치환된 구조에서 carborane이 보이는 삼차원 구조적 π-전자효과

김소연 BAQIANKAI[1] 최태섭[2] 강상욱[3,*]

고려대학교 세종캠퍼스 소재화학과 [1]고려대학교 과학기술대학 [2]고려대학교 세종캠퍼스 신소재화학과 [3]고려대학교 소재화학과

mono-phenyl 또는 di-phenyl o-carborane 을 출발물질로 하여 tri-phenylated 1,2,3-Ph_3?C_2B, 1,2,6-Ph_3?CB_2, tetra-phenylated 1,2,3,6-Ph_4?C_2B_2 을 37?86% 의 수득율로 합성하였다. 각 화합물의 결정구조를 통해 각 화합물에서 carborane 에서 C_2-C_2 사이의 거리가 각각 1.763, 1.632, 1.704 ? 임을 알 수 있었다. 전자끌개능력을 보이는 ortho-carborane 에서 phenyl 기의 개수와 위치를 조절함으로써 ortho-carborane 의 reduction potential 값을 조절할 수 있음이 밝혀졌다. DFT 계산결과 carborane 이 보이는 전자 받개 능력은 ortho-carborane 의 σ*-orbital 과 치환기의 π?orbital 과의 상호작용에 의해 나타나는 현상임을 알 수 있었다. 또한 치환기에 $Cr(CO)_3$ 를 도입함으로써 phenyl 기의 π?orbital 에 영향을 주어 그 영향을 관측한 결과 reduction potential 값을 더욱 positive shift 할 수 있었다.

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Synthesis of 1-O-alkylglycerides by methyl esters of vegetable oils for transformer oils

이성천 강은경[1] 이병민[2,*]

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Vegetable oils have some limits to use in the extreme conditions(high temperature, high pressure, long time use). To solve these problems, one of the ester bond of vegetable oils was converted into the ether bond which are more stable than ester groups. 1-O-alkylglycerides were synthesized by addition of 1-O-alkylglycerols to methyl esters of vegetable oils. The products were confirmed by GC, IR, and NMR. The pour point and viscosity of the products were tested as well.

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발표분야: 공업화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis and Characterization of Pt-Ru/Zeolite-templated Carbon for Direct Methanol Fuel Cells

임태진 박수진*

인하대학교 화학과

In this work, we prepared zeolite-templated carbon (ZTC) supports for direct methanol fuel cells (DMFCs). The ZTCs, which had high surface area and small pore diameter, were synthesized by conventional templating method. Pt-Ru catalysts were deposited onto ZTCs by chemical reduction method. The crystalline and structural features were investigated by X-ray diffraction (XRD). The textural properties of ZTC were investigated by N2/77 K adsorption isotherms using Brunauer-Emmett-Teller (BET) equation and Barret-Joyner-Halenda (BJH) method. The surface morphology was characterized by scanning electron microscope (SEM) and transmission electron microscopy (TEM). The electrochemical properties of Pt-Ru/ZTCs catalysts were also analyzed by cyclic voltammetry measurements.

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발표종류: 포스터, 발표일시: 수 16:00~19:00

Effect of Pore Structure on Electric Double Layer Capacitor Performance of Microporous Carbon

임태진 박수진*

인하대학교 화학과

In This work, we prepared the carbons from synthesized zeolite-templated carbon precursor. The prepared carbons were chemically activated, and then the activated zeolite-templated carbons were named as A-ZTCs. The activations were carried out at different temperatures to investigate the effect of activation temperature on the surface and electrochemical properties of the activated zeolite-templated carbons for using as an electrode of electric double layer capacitors (EDLC). The characteristics of A-ZTC were determined by X-ray diffraction (XRD), scanning electron microscopy (SEM), surface area and pore size analysis. Also, the electrochemical behaviors were observed by cyclic voltammetry and galvanostatic charge-discharge method.

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

Influence of KOH Activation on Electrochemical Behaviors of Pt-Ru/Microporous Carbons as Catalysts for Direct Methanol Fuel Cells

임태진 박수진*

인하대학교 화학과

In this work, microporous carbons were prepared by a conventional zeolite templating method using furfuryl alcohol for catalysts in direct methanol fuel cells (DMFCs). The zeolite template microporous carbons (ZTCs) were different KOH amounts, i.e., 0, 1, 2, 3 and 4g as an activating agent. The Pt-Ru metals were deposited onto activated ZTCs (A-ZTCs) by chemical reduction method. The characteristics of Pt-Ru ZTC catalysts were determined by specific surface area and pore size analyzer, X-ray diffraction (XRD), transmission electron microscopy (TEM). The textural properties of A-ZTC were investigated by N2/77 K adsorption isotherms using Brunauer-Emmett-Teller (BET) equation and Barret-Joyner-Halenda (BJH) method. The electrochemical properties of Pt-Ru/ZTCs catalysts were also analyzed by cyclic voltammetry (CV).

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

Silicon Carbide-loaded Pitch-carbornized Glass Fibers-reinforced composites for Thermal Conductivity

신용욱 박수진*

인하대학교 화학과

In this work, We prepared silicon carbide (SiC)-loaded pitch carbonized glass fibers-reinforced composites as a function of SiC amount. The surface properties were determined by fourier transform infrared (FT-IR) spectrometry analyses. The thermal properties of pitch-carbonized glass fibers-reinforced composites were investigated by differential scanning calorimetry (DSC) and laser flash diffusivity analyzer (LFA). Also, the mechanical properties were studied in fracture toughness by universal testing machine (UTM). As a result, these composites were explained that suitable amount of silicon carbide (SiC) played an important role in improving thermal conductivity.

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

Preparation and Characterization of ammonia-treated TiO2/polyethylene oxide Nanofibers by Electrospinning Technique

염대규 박수진*

인하대학교 화학과

In this work, ammonia-treated TiO2/polyethylene oxide nanofibers (A-TiO2/PEO NFs) were studied as a function of ammonia concentration. X-ray diffraction (XRD) and scanning electron microscopy (SEM) applied to determine the structure of A-TiO2/PEO NFs. Property of surface was characterized by X-ray photoelectron spectroscopy (XPS). And their photocatalytic properties of A-TiO2/PEO NFs were monitored through the photodegradation of methylene blue (MB) under visible light. As a result, the photocatalytic property of A-TiO2/PEO NFs was increased in comparison with the TiO2/PEO NFs due to the newly formed N-Ti-O bonds of A-TiO2/PEO.

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

Influence of KOH Activation on Hydrogen Storage Capacity of Rice Husks

유한진 박수진*

인하대학교 화학과

In this work, we have studied hydrogen storage capacity of KOH-activated rice husks derived carbon (RHC) synthesized under various conditions. We used rice husks as a carbon precursor. Rice husks were treated with different KOH ratios and carbonized at high temperatures (800, 900, 1000°C) in N2 condition. The surface morphology of RHC was examined by scanning electron microscopy (SEM). The structural properties of RHC were analyzed by X-ray diffraction (XRD). The specific surface area of RHC was investigated by Brunauer-Emmett-Teller (BET). Hydrogen storage capacity of RHC was measured by volumetric measurement at 77K/1 bar and 298K/100 bar. From this result, specific surface area was significantly increased after KOH activation. Hydrogen storage capacity difference was confirmed with KOH ratios and Temperatures.

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발표코드: **IND.P-109**
발표분야: 공업화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis of KOH-Activated Carbon Aerogels for Hydrogen Storage Capacities

유한진 박수진*

인하대학교 화학과

In this work, we prepared carbon aerogels for hydrogen storage. Carbon aerogels (CA) were synthesized using a soft-template method. KOH was used as an activation agent. CA was activated with KOH for different temperature and KOH ratios to figure out KOH activated CA for optimum conditions for hydrogen storage capacity. The surface morphology of KOH activated CA (KCA) was examined by scanning electron microscopy (SEM). The structural properties of KCA were investigated by X-ray diffraction (XRD). The specific surface area of KCA was analyzed by Brunauer-Emmett-Teller (BET). The hydrogen storage capacity of KCA was measured by volumetric measurement at 77K/1 bar and 298K/100 bar. This result highlights the importance of the structural and textural characteristics of the carbon aerogels, prepared at different activation temperatures on hydrogen storage capacity.

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

Synthesis and Characterization of Hydrous Manganse Oxides Composites

한인기 박수진*

인하대학교 화학과

In this work, the hydrous mangamese oxides (HMOs) are synthesized by alkaline permangnate solution and manganese (II) nitrate as a function of alkaline hydroxide. The surface morphology of HMOs was examined by scanning electron microscopy (SEM). The structural properties of HMOs were examined by X-ray diffraction (XRD). The textural properties were investigated by N2/77K adsorption isotherms using Brunauer-Emmett-Teller (BET) equation and Barret-Joyner-Halenda (BJH) method. The composition of HMOs were also analyzed by X-ray photoelectron spectroscopy (XPS). The ion adsorption efficiency of HMOs were also analyzed by using atomic adsorption spectroscopy (AAS).

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발표코드: **IND.P-111**
발표분야: 공업화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

산소센서용 백금 페이스트의 레올로지 특성 및 성능평가

구용환 이병철*

한국원자력연구소 방사선기기연구부

백금(Pt)은 초고온이나 산, 염기 분위기에서 강도가 우수하며 전기적, 촉매적 특성이 안정적으로 발현되는 소재로 다양한 센서의 촉매나 전극의 성분으로 적합한 재료이다. 하지만 가격이 비싸고 백금의 가공이 쉽지 않아 센서나 전극용도로 사용하는 백금은 페이스트로 제조하여 일정한 형태를 갖춘 패턴으로 만들어 사용을 한다. 현재 주로 사용되는 백금 페이스트는 마이크로급의 크기를 가지는 백금 입자를 사용하여 제조 하는데 이렇게 제조된 페이스트는 미세 선폭의 구현과 평활한 도막을 얻기 힘든 단점이 있다. 때문에 백금 나노입자를 사용하여 백금의 전기적, 촉매적 성질의 향상과 동시에 페이스트의 인쇄특성을 보완하여 개선된 센서소자용 재료로 각종 가스센서에 사용하고자 한다 따라서 (주)RTX 에서 합성된 백금 나노입자를 사용하여 아크릴계 레진과 유기용매의 종류와 함량에 따라 페이스트를 제조하였으며 레올로지에 따른 인쇄성 및 백금 패턴과 기판과의 접착성, 전기적 특성에 대한 물성을 연구하였다.

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

The development of eco-friendly biodegradable detergent

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The purpose of this study is developing low-toxic eco-friendly solvent so that it can replace conventional solvent cleaner in the fine chemical industry. Currently in use have many problems, such as VOC, toxic, low volatilization, biodegradable detergents. To use natural resources such as vegetable oil, the mixture of a carboxylic acid, alcohol can be used as a raw material, low toxicity and biodegradable detergent need to be developed. Biodegradation ability could solve the problems when leakage accident occurs because it will decomposed in the natural environment and doesn’t generate secondary pollution. We synthesized different kinds of detergents which is based of the nature to develop new detergent that features high detergency and biodegradation when the leakage accident is occurred.

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

Preparation of porous carbons from biomass and their application for the carbon capture

박서경 이제승*

경희대학교 화학과

Porous carbons derived from biomass (cellulose, chitosan, alginic acid) have been prepared by heat treatment under N_2 atmosphere and activating at high temperature under ammonia gas atmosphere. CO_2 adsorption capacities of prepared porous carbon materials and their dependence on the surface area and pore structure were investigated. Only by heat treatment, the surface areas of alginic acid were measured as 258.2 m^2 g^{-1} with a pore volume of 0.15 cm^3 g^{-1}. However, those values dramatically increased up to 1032.0 m^2 g^{-1} with a pore volume of 0.65 cm^3 g^{-1} after the activation process at high temperature under ammonia gas environment. The CO_2 adsorption capacity of ammonia activated carbon derived from alginic acid increased 1.48 to 2.20 mmol g^{-1}.

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

High value production and purification of MFB from industrial waste to available green resources

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Purpose of previous purification of MFB was not the recovery and use of MFB, but removal. This way not eco-friendly, but also generate a lot of industrial waste, so it causes environmental pollution. For more eco-friendly and re-usable process, MHB is synthesized by reaction of MFB with hydroxylamine and then, high-purity MFB is recovered by hydrolysis of MHB. High-purity MFB can be a precursor of pharmaceuticals, cosmetics, and polymer additives. First, we use high-purity MFB and synthesize Fluorescent Whitening Agent.

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발표코드: **IND.P-115**

발표분야: 공업화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Homogeneously catalyzed etherification of glycerol

권혁찬 정민석 이제승*

경희대학교 화학과

Glycerol has emerged as a significant worth bio-resource that can be converted into high valued materials such as plasticizer, food additive, and fuel additive, etc. The catalytic activity of different homogeneous catalysts was investigated during the etherification reaction of glycerol and the composition of products was evaluated using liquid chromatography. Alkali metal salts which have strong basicity showed high catalytic activity, indicated by high glycerol conversion with the corresponding selectivities of diglycerol, triglycerol, and oligomers of glyceol. The influences of various reaction variables including the nature of catalyst, the loading amount of catalyst, reaction time, and reaction temperature on the etherification of glycerol were also investigated.

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

저에너지 전자빔을 이용한 백금 나노입자의 형상 제어

임소연 채근석* 이임규[1]

(주)알티엑스 부설연구소 [1](주)알티엑스 기계장치부

전이 귀금속인 백금(Pt)은 우수한 촉매 특성과 전기적 특성, 그리고 뛰어난 내식성으로 화학, 석유화학, 제약, 전자, 자동차 산업에서 널리 활용되고 있다. 특히 강력한 촉매역할로 다양한 가스 센서에 응용되고 있으며 백금의 수요는 증가하게 되고 백금의 가격이 상승되는 요인이 될수 있다. 따라서 백금의 사용량을 줄이기 위해 대체 촉매 및 백금 촉매 저감 기술이 요구되고 있다. 이러한 일환으로 합금, 코어-쉘등의 구조로 합금화 하는 연구와 표면적을 극대화 하여 백금의 활성을 증가시키는 나노입자 합성 연구 등이 활발히 진행되고 있다. 일반적으로 백금 입자의 합성은 스퍼터증착법, 페치니법, 수열법, 콜로이드 합성법, 액상환원법등이 사용되고 있으며 본 연구에서는 화학적 환원제 대신 저에너지 전자가속기에서 발생되는 에너지로 강력한 환원에너지를 얻을수 있었다. 또한 용액의 농도, 반응 온도, 반응 시간과 같은 반응조건을 달리하여 백금 나노입자의 사이즈 및 형상을 제어할 수 있었으며 활성이 높고 촉매특성이 우수한 백금 나노입자를 제조할 수 있었다.

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발표종류: 포스터, 발표일시: 수 16:00~19:00

A Study on Thermal Conductivity of Silicon Carbide/Pitch-carbonized glass fiber composites

신용욱 박수진*

인하대학교 화학과

In this work, we prepared silicon carbide (SiC)-loaded pitch carbonized glass fibers-reinforced composites as a function of SiC amount. The surface properties were determined by Fourier transform infrared (FT-IR) spectrometry analyses. The thermal properties were investigated by differential scanning calorimetry (DSC) and laser flash diffusivity analyzer (LFA). Also, the mechanical properties were studied in fracture toughness by universal testing machine (UTM). As a result, these composites were explained that suitable amount of silicon carbide (SiC) played an important role in improving thermal conductivity.

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발표분야: 공업화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Carbon-coated silica aerogels as CO2 adsorbents

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경희대학교 화학과

Silica aerogels have been prepared using sol-gel method using the aqueous solutions of sugar as a template at an ambient temperature and pressure. Hydrogels were prepared from tetramethylorthosilicate (TMOS) under acidic condition by addition of formic acid. Carbon-coated silica aerogels were obtained successfully by carbonization of silica aerogel containing sugars at 800 oC and ambient pressure under nitrogen atmosphere. The pore structure of silica aerogels were successfully controlled by varying the molar ratio of sugar and TMOS. Carbon-coated silica aerogels have surface areas at a range of 0.6-350 m2 g-1 and show CO2 adsorption capacity at a range of 0.1-1.5 mmol g-1 at room temperature.

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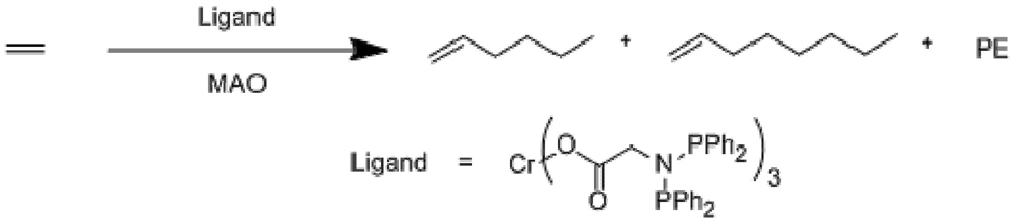
발표종류: 포스터, 발표일시: 수 16:00~19:00

고선택성의 ethylene tetramerization 촉매계 제조

박성연 이분열[*]

아주대학교 분자과학기술학과

1-옥텐은 대표적인 선형저밀도 PE 를 만들기 위한 단량체 또는 공당량체로서 중합공정에 광범위하게 사용되는 중요한 상업적 원료지만 전량 수입에 의존하고 있다. 우리나라 석유화학 생산 용량을 고려했을 때 1-옥텐의 생산을 위한 촉매 및 공정 개발이 절실히 요구된다. 에틸렌의 사량체화(tetramerization)를 통해 1-옥텐을 제조하는 P-N-P 골격의 크롬계 촉매가 Sasol 사에 의하여 2000 년대 초 개발되어 현재 생산 공정이 건설되고 있다. 국내에서는 2000 년대 후반, SK innovation 에서 P-C-C-P 골격의 리간드를 포함하여 이루어지는 크롬계 촉매를 제시하고 이 촉매를 이용하여 높은 순도의 1-옥텐을 제조할 수 있음을 보고하였다. 하지만 리간드 합성에 있어서 원료의 가격이 비싸고 반응 수율이 ~15% 수준밖에 못 미치기 때문에 상용화하는데 어려움이 있다. 따라서 본 연구에서 SK innovation 에서 개발한 P-C-C-P 골격 리간드의 새로운 합성 방법을 개발하고, 더불어 새로운 P-N-P 골격 리간드를 합성하였다.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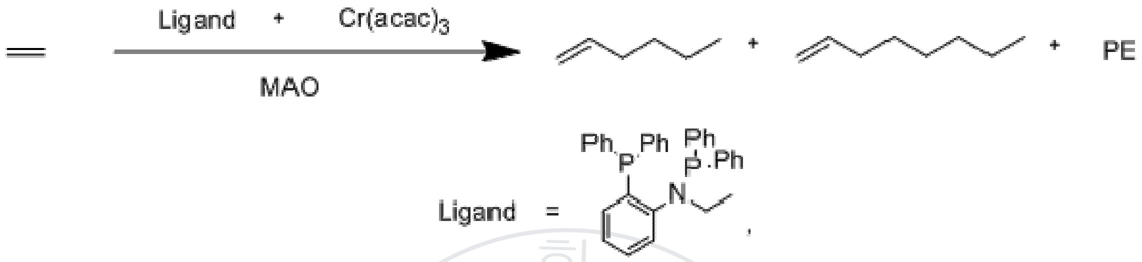
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Ph
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일시: 2014년 4월 16~18일(수~금) 3일간
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The effective synthesis of polymeric sulfur using Electron beam

조보배 유국현*

동국대학교 화학과

Rubber products for the applications in various industries such as automatives, hose, shoes, etc s will be considered. Rubber vulcanization is the most important process in manufacturing rubber product. However,, if you use normal sulfur - processed rubber products have the problem as blooming occurs.To solve this problem, we should use polymeric sulfur. polymeric sulfur is an essential factor to make rubber products with better quality and performancesCurrent synthesis method for polymeric sulfur has economic, environmental and safety issues since the process is caused by the high thermal polymerization and the use of carbon disulfide. Carbon disulfide is well known as toxic solvent.Synthesis of polymeric sulfur using the electron beam will be regarded as a innovative methods Electron beam irradiation process for the synthesis of polymeric sulfur does not required the use of solvent and high thermal polymerization process, it will be a promissing approach to solve many problems from conventional rubber industry.

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Preparation and characterization of NIR absorbed antimony doped tin oxide polymer film

이원길 유국현*

동국대학교 화학과

From tens to hundreds of nanometer-sized metal oxides are known to absorb in the near-infrared (700-2500nm) region. The energy absorption at wavelengths of the near infrared region by antimony doped tin oxide (ATO) is excellent, and the transparent properties of the nano-sized particles used to form transparent windows favor their use as a heat protecting material. NIR absorption by ATO was optimized with respect to the antimoney dopant. ATO can be used as a coating agent in applications such as heat protecting funtionalised glass panels or transparent plastic materials. The polymer matrix coating agents could be formed via the crosslinking reaction of silanol monomer or oligomers, dilutes, and silica sols. The thermal stability, mechanical and optical properties were investigated. Structural and morphological features of coatings were assessed using Fourier transform infrared spectroscopy (FTIR), and transmission electron microscopy (TEM). Performance of the coatings was evaluated using water resistance studies, thermo-gravimetric analysis (TGA) and heat-absorbing ability such as surface temperature, increasing of inner chamber temperature. The data showed that the ATO coatings possessed good mechanical properties and thermal stability. The UV?visible?near infrared (UV?VIS?NIR) spectra results suggested that the ATO coatings could absorb near infrared radiation so that it would prevent heat transmission and heat diffusion effectively.

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발표종류: 포스터, 발표일시: 수 16:00~19:00

water desalination plant and system for the production of pure water and salt

장다영[*] 김종부[1] 이장훈 서항복[2]

(주)에스이씨 기업부설연구소 [1](주)해동테크놀로지 기업부설연구소 [2](주)해동테크놀로지 대표이사

The present study discloses a desalination plant that operates with a Salt-containing waste water or brackish water feed and produces a concentrated and selectively improved salt reject stream and a pure water permeate stream from a first treatment section that is arranged to produce primarily water at high recovery using membrane desalination processes. The reject stream from the first treatment line has a component distribution that is substantially reduced in native di-and polyvalent scaling ions, essentially depleted of sulfate, has substantially higher total dissolved solids than a traditional sea water reverse osmosis reject, yet is suitable for thermal treatment processes. The system may be enhanced by monovalent salt components. The unit may be integrated with a second treatment section, in which the first reject stream is further concentrated, purified, and processed to produce a high purity salt product.This research was supported by the Program for the Construction of Eco Industrial Park(EIP) which was conducted by the Korea Industrial Complex Corporation(KICOX) and the Ministry of Knowledge Economy (MKE)

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Reduced fouling of reverse osmosis membranes

장다영* **김종부[1]** **이장훈** **서항복[2]**

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The present study provides a new water purification method and system using reverse osmosis. Colloidal fouling of RO elements can seriously impair performance by lowering productivity and sometimes salt rejection. An early sign of colloidal fouling is often an increased pressure differential across the system. The source of silt or colloids in reverse osmosis feed waters is varied and often includes bacteria, bacteria, clay, colloidal silica, and iron corrosion products. Pretreatment chemicals used in a clarifier such as aluminum sulfate, ferric chloride, or cationic polyelectrolytes are materials that can be used to combine these fine particle size colloids resulting in an agglomeration or large particles that then can be removed more easily by either media or cartridge filtration. In particular, the present study provides methods and water purification systems using an ion exchange resin and absorbent media for pretreatment of water being fed to a reverse osmosis treatment system, where the pretreatment reduces fouling of, or deposits or chemical attack on the membrane surfaces and passageways. Particularly, a macroporous resin having an average pore diameter in the range of 1,000 to 500,000 Angstroms and a crush strength or Chatillon value of at least 24 g/bead (710 μm bead diameter) is used.This research was supported by the Program for the Construction of Eco Industrial Park(EIP) which was conducted by the Korea Industrial Complex Corporation(KICOX) and the Ministry of Knowledge Economy (MKE)

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

Preparation and properties of copper oxide catalyst impregnated non-woven fabric filters

장다영* 김종부[1,*] 이장훈 서항복[2]

(주)에스이씨 기업부설연구소 [1](주)해동테크놀로지 기업부설연구소 [2](주)해동테크놀로지 대표이사

A catalyst with CuO non-woven fabric filter for treatment of VOC was prepared and characterized. Catalytic filter can not only potentially achieve the substantial savings in energy but provide with effective optimization and integration of process for removal of VOC from indoor air. Preparation of catalyst impregnated non-woven fabric filter with disk shape follow the processing of alumino-silicate ceramic filter, support impregnation and catalyst impregnation (copper oxide). Preparation routes of alumino-silicate catalyst carrier suitable for production of catalytic filters practically were studied and developed using the sol-gel and colloidal processing, homogeneous precipitation and impregnation method. Characterization of the catalyst, catalyst carrier catalytic filter materials have been performed the using various techniques such as BET, XRD, TGA, SEM. Combination of the sol-gel and colloidal processing and impregnation method is recommended to prepare catalyst carriers economically for catalytic filter applications.

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Suzuki-Miyaura cross-couplings of (π-allyl)Pd cationic complexes containing a NHC(N-heterocyclic carbene) ligand

김용주* 최근영 최준환 박수진[1] 이순원[1]

강릉원주대학교 화학과 [1]성균관대학교 화학과

Various (π-allyl) Pd cationic complexes having NHC ligands were obtained from the reactions of (π-allyl) Pd chlorides with 1 equiv. of AgBF4. Also, cleavage reactions of bis(π-allyl) Pd chlorides with chealted phosphines produced chelated phosphine-bridged dinuclear (π-allyl) Pd chloride. Then, treatment with AgBF4 or AgoTf afforded (π-allyl) Pd cationic complexes with a chelated phosphine. The isolated complexes were characterized by spectroscopic analyses and some of X-ray diffraction study. Also, Suzuki-Miyaura cross C-C coupling reactions using the some of various (π-allyl) Pd ionic complexes underwent.

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Pd-S and Pd-N bond formation from dialkyl Pd(II) and-Pt(II) complexes using organic pseudo halides

김용주* <u>이선계</u> 박수진[1] 이순원[1]

강릉원주대학교 화학과 [1]성균관대학교 화학과

Reactions of trans-PdEt2L2 (L=PMe3,PEt3,PMe2Ph) with various organicisothiocyanates (R?NCS) afforded corresponding dithiocarbonimidato Pd(II) complexes {L2Pd[S2C=N-(R)]}complexes, depending on the isothiocyanates. Treatments of {(Me3P)2Pd[S2C=N-(R)]}(R-(-) and S-(+)) with a chelated phosphine such as 1,2-bis(diethylphosphino)ethane = DEPE and 1,2-bis(dimethylphosphino) ethane = DMPE) readily afforded corresponding chelated complexes, {(L~L)Pd[S2C=N-(R)]}(R-(-) and S-(+)) in high yield. Reactions of trans-MEt2L2(M = Pd, Pt; L= PMe3, PEt3, PMe2Ph) with organic isothiocyanates(R-NCS; R = Benzyl, Et) or thiocyanates (R-SCN; R=Benzyl, Et) were investigated. Also, similar reactions with R-NCO (R = Ph, Tolyl) were examined. Experimental details will be discussed.

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

Synthesis and properties of Pd(II) trifluoroacetates containing mono or bis chelated phosphines

김용주* 김건우 박수진[1] 이순원[1]

강릉원주대학교 화학과 [1]성균관대학교 화학과

Transition metal carboxylates are extensively investigated because of versatile coordination modes such as unidentate, chelate, and symmetrical or asymmetrical bridging coordination on the carboxylate oxygen atom. The trifluoroacetate group is well known for their contribution to the solubility or electronic property of the organic substrate in the transition metal-catalyzed organic reactions. However, there have been limited number of studies about the synthesis and chemical properties of group 10 metal trifluoroacetates. In this work we prepared various Pd(II) trifluoroacetates containing mono or bis chelated phosphines from ligand substitution using dmpe, depe, dppf, dippf and then applied to transition metal -catalyzed reactions.

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발표분야: 무기화학

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Triarylboryl Substituted Oxadiazole as Multi-functional Materials in Green PhOLEDs

<u>NGUYEN VAN NGHIA</u> 박지현 이민형*

울산대학교 화학과

2,5-Bis-(m-dimesitylboryl-phenyl)-1,3,4-oxadiazole compound (1) was prepared and characterized to investigate multi-functional properties in phosphorescent OLEDs (PhOLEDs). X-ray crystal structure shows that two Mes_2B groups are oriented towards the same side. From optical properties and cyclic voltammetry measurements, 1 was found to be suitable for electron transporting (ETL) and/or host materials in PhOLEDs. Green PhOLED devices incorporating 1 as ETL, host, or ETL with host were fabricated and compared their performance with that of the well-known CBP (9,9'-(1,1'-biphenyl)-4,4'-diylbis-9H-carbazole) based devices. Among them, the devices based on 1 as host show high performane that is even comparable to that of CBP based devices. Details of synthesis, characterization, and multi-functional properties in PhOLEDs of 1 will be discussed.

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발표분야: 무기화학
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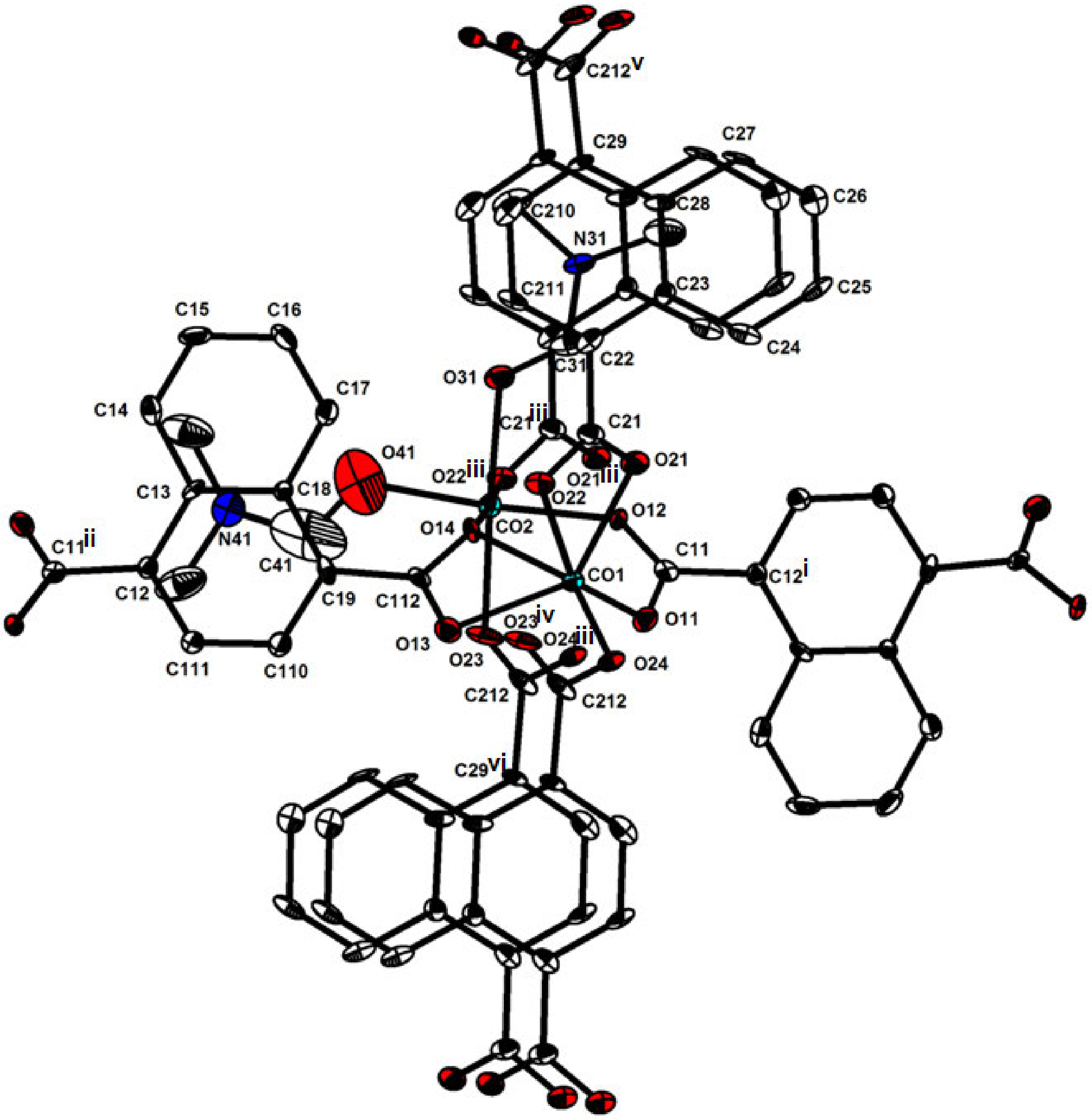
Three-Dimensional Cobalt(II) and Cadmium(II) MOFs Containing 1,4-Naphthalenedicarboxylate

최인환 김영미[1] 이도남[2,*] 허성[*]

한국외국어대학교 화학과 [1]이화여자대학교 나노바이오 기술연구소,화학-나노과학과 [2]광운대학교 화학과

Three-dimensional (3D) cobalt(II) and cadmium(II) metal-organic frameworks bearing rigid 1,4-naphthalenedicarboxylate (1,4-NDC) linkers were prepared and their solid-state structures were characterized by single crystal X-ray diffraction analysis. Both Co-MOF and Cd-MOF exhibited isostructural frameworks. 1,4-NDC ligands bridge the metal ions in chelating/bridging and simple bridging modes to form a 1D chains, and these 1D chains are interconnected by 1,4-NDC ligands to form 3D frameworks with the formula of $[M_2(1,4\text{-NDC})_2(DMF)_2]$ (M = Co^{II} or Cd^{II}). Two asymmetric metal ions have different coordination geometries: one adopted octahedral geometry bound by four carboxylate oxygen atoms and two DMF oxygen atoms, and the other adopted pseudo-tetrahedral geometry bound by two chelating carboxylates and two carboxylate oxygen atoms. Two mutually *cis*-positioned DMF ligands could be thermally removed under vacuum to lead to MOFs with openly accessible Lewis acidic metal sites. Despite the nonporosity of the framework after the removal of DMF ligands, the as-prepared Cd-MOF was found to be catalytically active for the cyanosilylation reaction of aromatic aldehydes with nitro substituent in varying positions in the presence of trimethylsilyl cyanide to afford cyanohydrin trimethylsilyl ethers in a shape and size selective manner. The reaction is thought to have mainly occurred inside the Cd-MOF micropores, where openly accessible coordination sites are available once the labile DMF ligands dissociate from Cd ions in solution.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C27
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C210
C28
N31
C211
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C16
C22
C31
C24
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O31
C14
C21iii
C21
O41
O21
O22iii
O21iii
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O22
O12
CO2
O14
N41
C11ii
C11
C41
CO1
C12i
C12
C19
C112
O11
O23iv
O24iii
O13
O23
O24
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C110
C212
C212
C29vi

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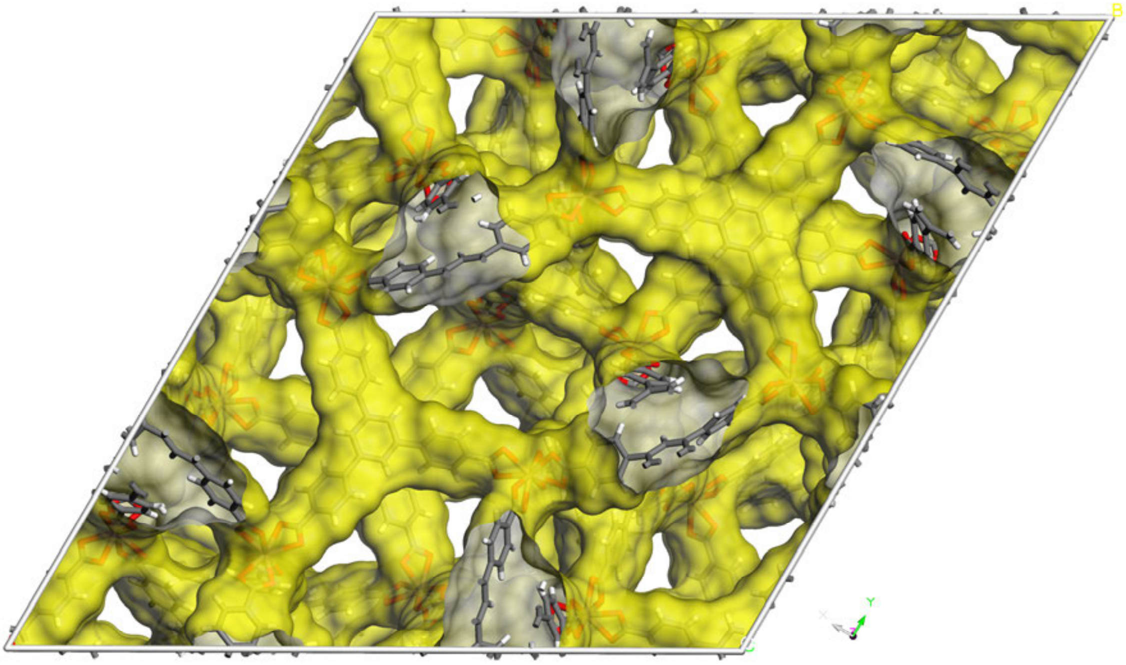
Efficient Encapsulation of Various Guests by Anionic In-MOF Containing Tritopic BTB Ligand

조은영 허성[*] 김성진[1] 김영미[2,*]

한국외국어대학교 화학과 [1]이화여자대학교 화학과 [2]이화여자대학교 나노바이오 기술연구소, 화학-나노과학과

New In^{III}-metal organic framework (In-MOF) having a large void volume was prepared and structurally characterized by single crystal X-ray diffraction. Thermal reaction between the tritopic ligand, 1,3,5-benzenetribenzoic acid (H_3BTB), and $In(NO_3)_3$ hydrate in diethylformamide yielded colorless crystals formulated as $[(CH_3CH_2)_2NH_2]_3[In_3(BTB)_4] \cdot 10DEF \cdot 14H_2O$ (1). The counter-cation and solvent-free doubly interpenetrated 1 contains 69.8% of solvent accessible void space. The framework of 1 was not stable enough to maintain its original structure when the solvent molecules were completely removed under vacuum. Despite this nonporosity due to the framework unstability, the as-prepared 1 was found to be a very good sorbent material for positively charged acridine orange hydrochloride, a large Reichardt's dye, and hydrophobic iodine molecule in solution. The time-dependent encapsulation kinetics of these guest molecules was investigated. The as-prepared 1 exhibited the increased uptake amount in the order of Reichardt's dye > acridine orange hydrochloride > iodine. The largest uptake of bulky Reichardt's dye by 1 could be attributed to the strong interaction between large aromatic-rich void space of 1 and Reichardt's dye. The structure of Reichardt's dye-encapsulated 1 was unambiguously characterized by X-ray crystallography.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일시: 2014년 4월 16~18일(수~금) 3일간
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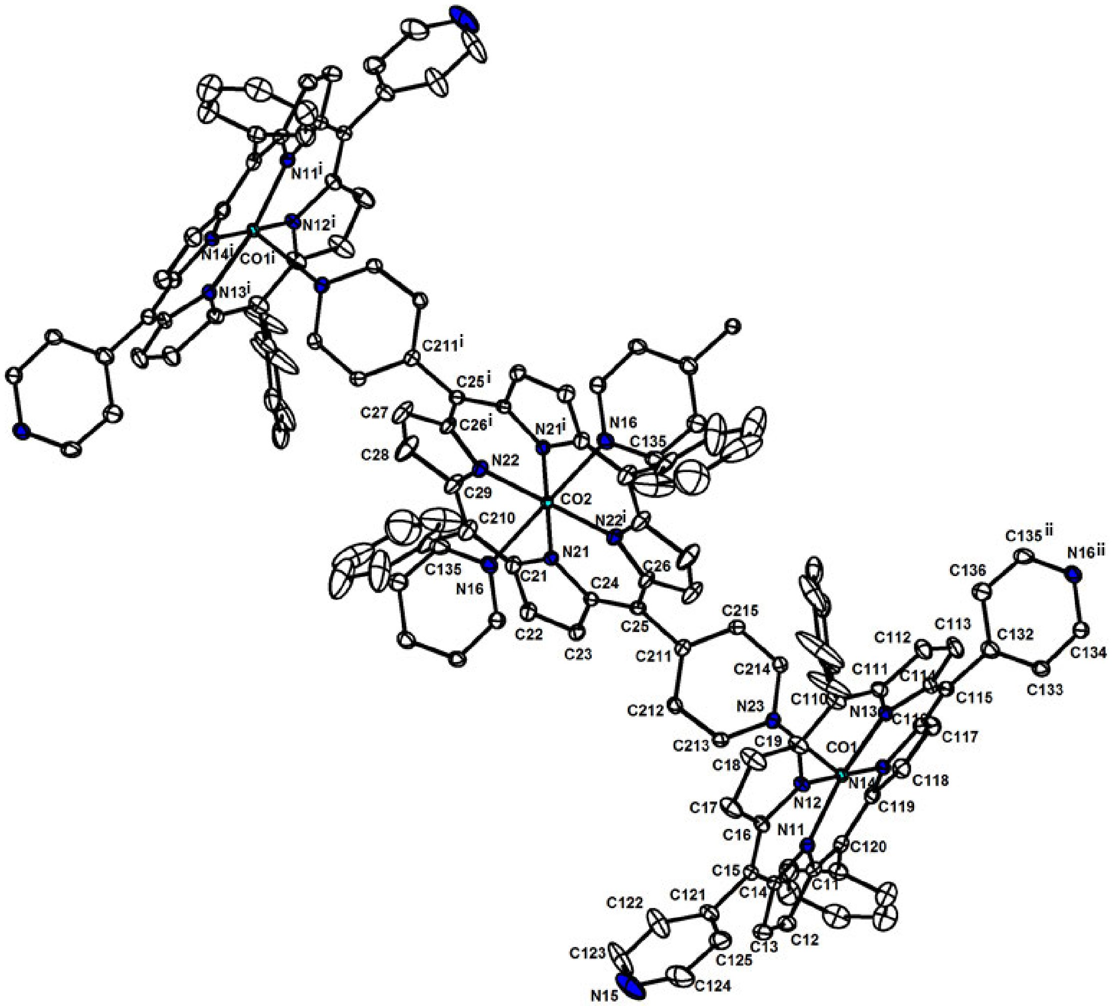
CO_2 Selective 1D Double Chain Dipyridyl-Porphyrin Based Porous Coordination Polymers

김현철 이영선[1] 허성[*] 이석중[1,*] 김영미[2,*]

한국외국어대학교 화학과 [1]고려대학교 화학과 [2]이화여자대학교 나노바이오 기술연구소,화학-나노과학과

Thermal reactions of MnCl(DPyP) (DPyP = 5,15-di(4-pyridyl)-10,20-diphenylporphyrin) as a metalloligand with Co^{II} and Zn^{II} ions in dimethylformamide led to neutral one-dimensional (1D) double chain dipyridyl-porphyrin-based porous coordination polymers (PCPs), $Co_3(DPyP)_3$ · 4DMF (1) and $Zn_3(DPyP)_3$ · 2DMF · $4H_2O$ (2). Both PCPs were structurally characterized by X-ray crystallography. Particularly, the central Mn^{III} ion in MnCl(DPyP) was transmetallated with Co^{II} or Zn^{II} ions and the central Co^{II} or Zn^{II} ions were further coordinated to pyridyl groups of neighboring M(DPyP) (M = Co or Zn) porphyrin complexes. PCPs 1 and 2 are isostructural and each 1D double chain interacts with another 1D double chain by multiple hydrogen bonding to stabilize the resultant framework. Therefore, solvent-free 1D double chain PCPs have permanent porosity, and the void volumes of the solvent-free 1 and 2 are calculated to be 22.6% and 23.0%, respectively. Gas sorption analysis indicated that 1 and 2 exhibited selective adsorption of CO_2 at 196 K. Both PCPs exhibited much smaller sorption abilities for N_2 (77 K), H_2 (77 K), and CH_4 (196 K) than CO_2 (196 K). Both PCPs exhibited different PXRD patterns when dried at 373 K, which indicated that the framework transformation of the isostructural $M_3(DPyP)_3$ type of PCPs strongly depended on the type of central metal ions.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C213
C19
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발표종류: 포스터, 발표일시: 수 16:00~19:00

Calix[4]arene-based Metallosupramolecular Architecture Controlled by the Lengths of Alkyldiammonium Guests

이은지 주희영 박기민*

경상대학교 화학과

Our interest in the development of metallosupramolecular architecture with cavities controlled by guest molecules has led us to investigate the coordination polymers based on calix[4]arene derivatives, in which metal ions link the calix unit to give the network with the cavities accommodating several guest species. To realize our idea, we employed a low rim-functionalized calix[4]arene tetraacetic acid (H_4CTA) with 1,3-alternative conformation as a multidentate building block and diaminoalkanes as the guest molecules. In the solvothermal reaction of H_4CTA and Zn(II) ion in the presence of alkyldiamines, as expected, two types of new metallosupramolecular architectures based on calix[4]arene tetraacetate (CTA^{4-}) depending on the lengths of α,ω-alkyldiammonium guests $^{+}NH_3\text{-}(CH_2)_n\text{-}NH_3^{+}$ (n = 2-4 and 6-10) have been synthesized by including suitable organic dication guests. Their single-crystal X-ray diffraction analysis reveal that the short organic dication guests (n = 2-4) lead to form two-dimensional framework with the cavity consisting of two CTA^{4-} and four Zn(II) ions whereas the long organic dication guests (n = 6-10) give rise to generate three-dimensional network with the cavity surrounded by six CTA^{4-} and four Zn(II) ions. The organic dication guests in both metallosupramolecular architectures are well accommodated by cavity via a variety of supramolecular interactions including electrostatic interactions, hydrogen bonds and van der Waals interactions. We will present and discuss a study on the syntheses and characterization of two new calix[4]arene-based metallosupramolecular architectures with the cavities controlled by the lengths of alkyldiammonium guests.

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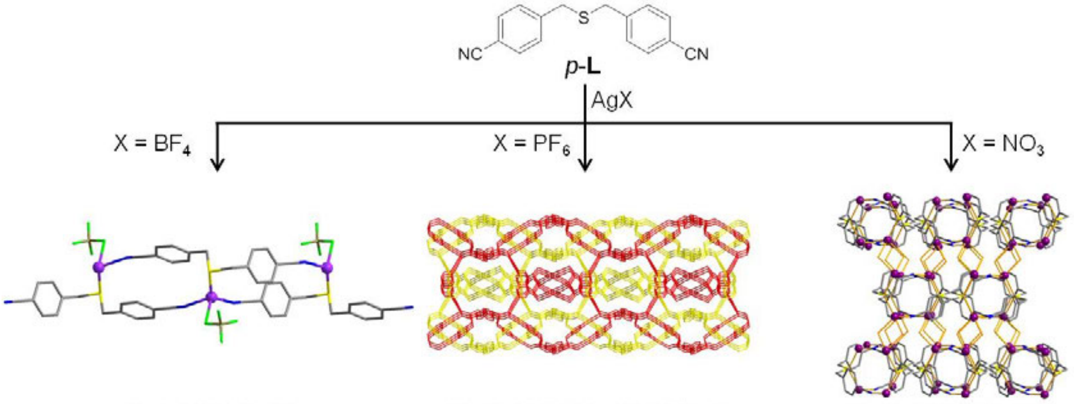
Anion-Dependent Coordinative Networking of Bis(cyanobenzyl)sulfide with Silver(I) Ion

이은지 박기민* 이심성*

경상대학교 화학과

Ligand isomers (*o*-L, *m*-L and *p*-L) of bis(cyanobenzyl)sulfide were employed as building blocks and their supramolecular silver(I) complexes are reported. The reactions of *o*-L, *m*-L, and *p*-L with silver(I) salts (X = BF_4^-, PF_6^-, or NO_3^-) afforded the respective anion-dependent complexes 1-10 with different topologies. For examples, the reactions of *o*-L with $AgBF_4$ and $AgPF_6$ afforded an anion-noncoordinated loop-type 1D coordination polymer $\{[Ag(o\text{-}L)](X)\}_n$ (1: X= BF_4^- and 2: X= PF_6^-). On the other hand, the reactions of *o*-L with $AgNO_3$ afforded an anion-coordinated loop-type 1D coordination polymer $[Ag(o\text{-}L)(NO_3)]_n$ (3). The reactions of *m*-L with $AgBF_4$ and $AgPF_6$ yielded isostructural 1D zigzag polymers of type $\{[Ag(m\text{-}L)](X)\}_n$ (4: X= BF_4^- and 5: X= PF_6^-). The reaction of *m*-L with $AgNO_3$, supramolecular isomers 6 and 7 of type $[Ag_2(m\text{-}L)(NO_3)_2]_n$ with different 2D network structures were obtained depending on the molar ratios of reactants. Meanwhile, the reaction of *p*-L with $AgBF_4$ afforded a double-stranded 1D coordination polymer $[Ag(p\text{-}L)(BF_4)]_n$ (8). Treatment of *p*-L with $AgPF_6$ and $AgNO_3$ afforded a 2-fold interpenetrated 3D Network $\{[Ag_3(p\text{-}L)_4](PF_6)_3\cdot 4CH_2Cl_2\}_n$ (9) and a multichannel 3D framework $[Ag_2(p\text{-}L)(NO_3)_2]_n$ (10), respectively.



$[Ag(p\text{-}\mathbf{L})(BF_4)]_n$ (**8**)
Double-Stranded 1D Polymer

$\{[Ag_3(p\text{-}\mathbf{L})_4](PF_6)_3\cdot 4CH_2Cl_2\}_n$ (**9**)
Interpenetrated 3D Network

$[Ag_2(p\text{-}\mathbf{L})(NO_3)_2]_n$ (**10**)
Multichannel 3D Network

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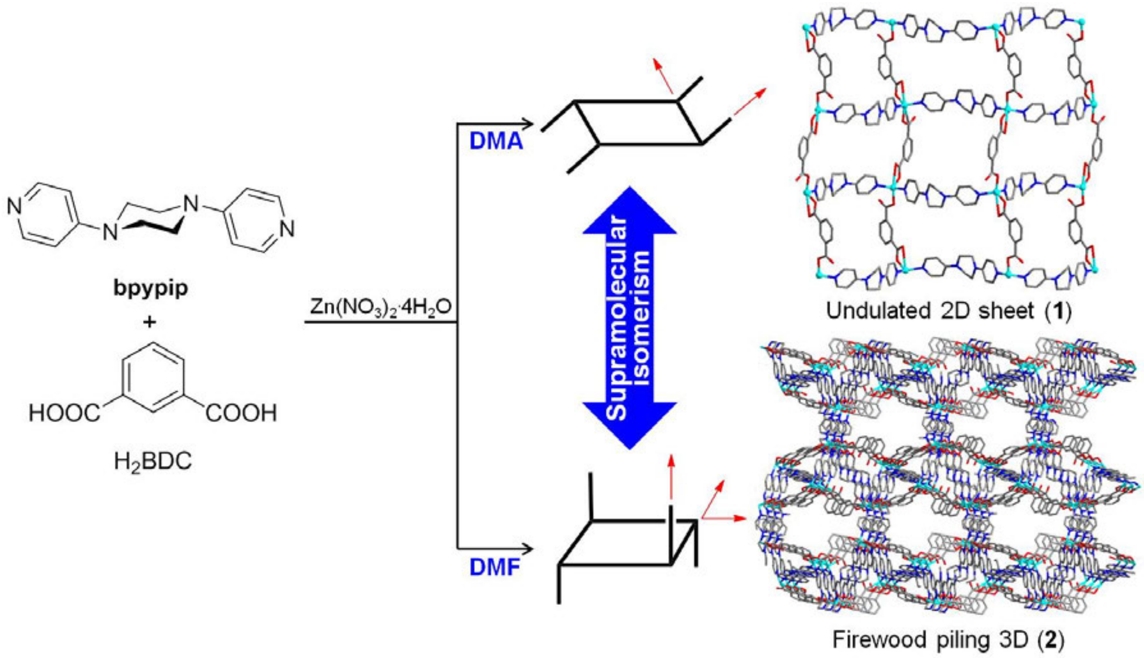
Supramolecular Transition Metal Complexes with 1,4-Bis(4-pyridyl)piperazine and Angular Dicarboxylic Acid

주희영 박기민* 이심성*

경상대학교 화학과

The intrinsic semi-flexibility of 1,4-bis(4-pyridiyl)piperazine (bpypip), associated with its bidentate and multidirectional binding functionality, can provide excellent potential for the construction of the new types of coordination frameworks. In connection with this reason, bpypip was chosen as organic building blocks. Binary ligand system of bipyridine derivative and aromatic carboxylic acids (H_2BDC and H_2pydc) was employed to prepare metal-organic frameworks (1-5). First, the reaction of bpypip, $Zn(NO_3)_24H_2O$, and H_2BDC in DMA yielded a grid-type 2D network $\{[Zn_2(bpypip)_2(BDC)_2]\cdot 4DMA\cdot 6H_2O\}_n$ (1). Interestingly, when DMF was used instead of DMA, $\{[Zn_2(bpypip)_2(BDC)_2]\cdot 4DMF\cdot 4H_2O\}_n$ (2) adopting a 3D channel structure was isolated as a supramolecular isomer of 1 (*see below*). In the reaction of bpypip with $Cu(NO_3)_2\cdot 3H_2O$ in the presence of H_2BDC, a 2D network $\{[Cu(bpypip)(BDC)]\cdot 2DMA\}_n$ (3) in which the Cu(II) and BDC form a 1D double chain and further doubly linked by bpypip in the axial positions. The reaction of bpypip with $Cu(NO_3)_2\cdot 3H_2O$ in the presence of H_2pydc resulted in the formation of dumbbell-like complex $[Cu_2(bpypip)_2(pydc)_2]$ (4). In addition, the reaction of bpypip with $Co(NO_3)_2\cdot 6H_2O$ in the presence of H_2pydc gave slip-stacked-brick type 1D polymer $\{[Co_2(bpypip)_3(pydc)_2]\cdot 4H_2O\}_n$ (5). Notably, the two different conformation of bpypip which are the quasi-linear and bent-type were existed in 5.



bpypip
+
H_2BDC
HOOC
COOH
$Zn(NO_3)_2 \cdot 4H_2O$
DMA
DMF
Supramolecular isomerism
Undulated 2D sheet (**1**)
Firewood piling 3D (**2**)

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Soft and Hard Metal Complexes of an O_4S_2-Macrocycle:Single-Crystal X-ray and NMR Studies

류현수 박기민 이심성*

경상대학교 화학과

An O_4S_2-macrocycle L was synthesized and structurally characterized by X-ray analysis. The X-ray crystal structures of five complexes (1-5) have been determined, and a range of structural types and coordination modes, including discrete to continuous forms, mono- to multinuclear, and endo- to exocyclic structures involving M-S and M'-O bonds are presented. Reaction of L with $Pb(ClO_4)_2$ yielded the endocyclic mononuclear lead(II) complex $[PbL(ClO_4)_2]$ (1). Reactions of L with silver(I) nitrate afforded the exocyclic dimer $[Ag_2L_2(NO_3)_2]$ (2). In the disilver complex 2, two macrocycles are linked with an Ag-(μ^2-NO_3)$_2$-Ag square-unit. Furthermore, the reaction of L with CuI gave a mixture of an exocyclic monomer [CuLI] (3, brick-shape) and an exocyclic dimer $[(Cu_2I_2)L_2]$ (4, rhomboid-shape) with two different shapes. From the mixture, 3 and 4 were separated under the microscope and confirmed separation with PXRD patterns. The straightforward one-pot reaction of L with CuI in the presence of NaI resulted in the heteronuclear endo/exocyclic complex $[Na_2(\mu_4\text{-}Cu_6I_8)L_2(CH_3CN)_4]_n$ (5). In 5, the endocyclic macrocyclic Na^+ complex units are linked by the twisted ribbon-type cluster $[Cu_6I_8]^{2+}$ resulting in the unique 2D network. In addition, the NMR titration was carried out in CD_3CN to understand further structural characteristic of the Ag^+ complex in solution. Upon stepwise addition of Ag^+, every proton in ligand shifted, suggesting the stable complexation for the fast exchanging system. The NMR titration curves clearly show an inflection point at mole ratio (Ag^+/L) of 1.0, indicating that the stoichiometry for the formation of the complex is also 2:2 ratio (metal to ligand).

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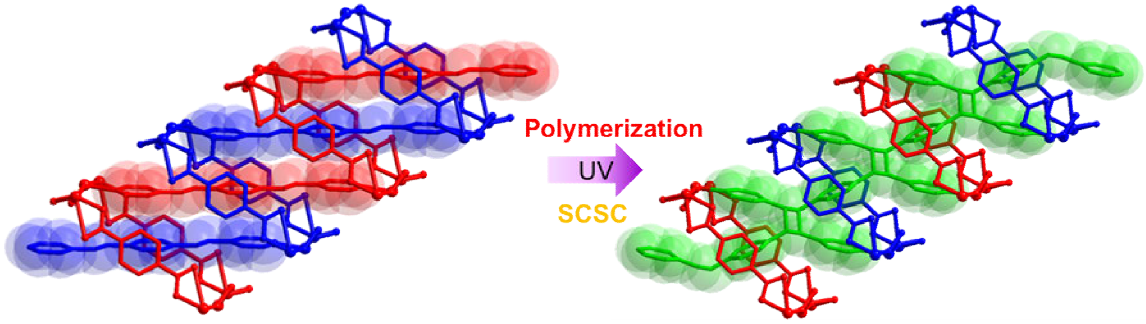
Single-Crystal to Single-Crystal Transformation of a MOF to a Metal-Organo Polymeric Framework (MOPF) via Photo-Induced Cycloaddition Reaction

박인혁 Anjana Chanthapally[1] 이형환 Hong Sheng Quah[1] 이심성[*] Jagadese J. Vittal[1,*]

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

Recently we have reported that the metal complex of an organo polymer ligand can be obtained indirectly by the [2+2] cycloaddition reaction in the solid state.[1] In this case, the organic polymer containing cyclobutane rings has been incorporated into a MOF using 1,4-bis[2-(4'-pyirdyl)ethenyl]benzene (bpeb). The observed polymerization is possible because of the infinitely slip-staked conjugated C=C bonds of the bpeb ligands forming a plane in the MOF. In the present study, the bpeb ligands aligned in a slip-stacked manner in a two-fold interpenetrated MOF 1, [Zn_2(bpeb)(bdc)$(fa)_2$] (bdc = 1,4-benzenedicarboxylate, and fa = formate) undergo [2+2] cycloaddition reaction via single-crystal to single-crystal (SCSC) manner to a MOPF 2, [Zn_2(poly-bppcb)(bdc)$(fa)_2$] (*poly*-bppcb = 1,3-(4,4'-bipyridyl)-2,4-phenylene-cyclobutane) (*see* below). The 3D structure has a 2D coordination polymer [Zn_2(bdc)$(fa)_2$] fused together with an *poly*-bppcb, to give a new MOPF structure which is unlikely to be synthesized by any other means so far.

Reference1. I.-H. Park, A. Chanthapally, Z. Zhang, S. S. Lee, M. J. Zaworotko, J. J. Vittal, *Angew. Chem. Int. Ed*. 2014, *53*, 414?419.



2-Fold interpenetrated Zn(II) MOF **1**
with a rotaxane structure

Zn(II) MOPF **2**
with a polyrotaxane structure

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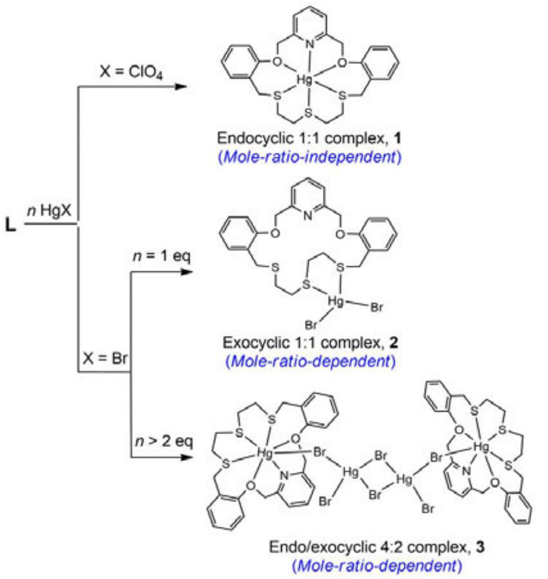
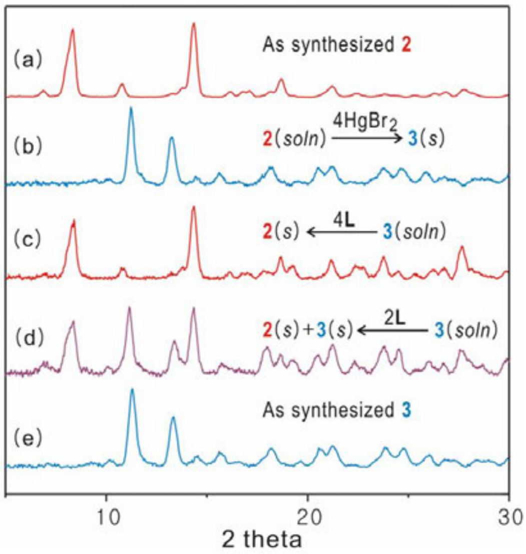
Anion and Mole-Ratio Effects on the Formation of Supramolecular Complexes of an NO_2S_3-Macrocycle

이형환 박인혁 이심성*

경상대학교 화학과

Synthesis of an NO_2S_3-macrocycle (L) incorporating a pyridine subunit and its anion and/or mole-ratio-dependent coordination modes in the formations of mercury(II) complexes are reported. When the mercury(II) salts with different anions (ClO_4^- or Br^-) were reacted with L, the $Hg(ClO_4)_2$ afforded a typical endocyclic complex $[HgL](ClO_4)_2$ (1). Meanwhile, the $HgBr_2$ gave an exocyclic complex $[HgLBr_2]$ (2) in which the metal ion exists outside the macrocyclic cavity. The observed anion effect on the coordination modes can be explained by the anion coordination ability toward the metal cation. In the mole-ratio variation experiments, notably, the use of 1.5 equiv or above amount of $HgBr_2$ in the same reaction condition gave a unique endo/exocyclic dumbbell-type complex 3, $[Hg_4L_2Br_6][Hg_2Br_6]$. However, the formation of the endocyclic $Hg(ClO_4)_2$ complex 1 shows no mole-ratio dependency. To monitor the observed mole-ratio-dependent exo-coordination products as well as their reactivities and reversibility, the systematic powder X-ray diffraction (PXRD) analysis has also been applied (see below). From the single crystal X-ray and the PXRD analyses, it was found that the endocyclic complex 1 is inert, but the complexes 2 and 3 have the liable nature and the reversibility between them in the presence of the corresponding reactants.


L
n HgX
X = ClO$_4$
X = Br
n = 1 eq
n > 2 eq
Endocyclic 1:1 complex, **1**
(*Mole-ratio-independent*)
Exocyclic 1:1 complex, **2**
(*Mole-ratio-dependent*)
Endo/exocyclic 4:2 complex, **3**
(*Mole-ratio-dependent*)


(a) As synthesized 2
(b) 2(soln) 4HgBr$_2$ → 3(s)
(c) 2(s) ← 4L 3(soln)
(d) 2(s)+3(s) ← 2L 3(soln)
(e) As synthesized 3
10
20
30
2 theta

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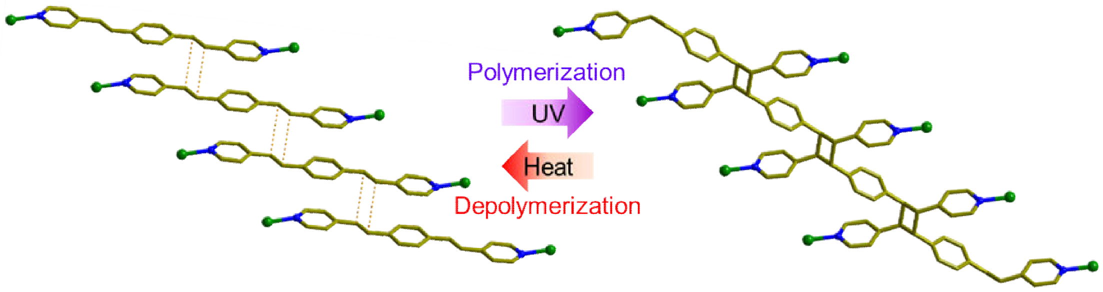
Metal-Assisted Formation of a Metal-Organo Polymeric Framework (MOPF) by Photo-Induced Cycloaddition Reaction and Its Thermal Cleavage

박인혁 Anjana Chanthapally[1] Zhenjie Zhang[2] 이심성[*] Michael J. Zaworotko[2,*] Jagadese J. Vittal[1,*]

경상대학교 화학과 [1]Department of Chemistry, National University of Singapore, Singapore [2]Department of Chemistry, University of South Florida, USA

Blending the organic polymers into the MOFs may combine the structural regularity of the metal containing MOFs and the unique properties of the organic polymers to produce new and better functional hybrid materials. Here we describe a new hybrid material that contains an organic polymer, 1,3-(4,4’-bipyridyl)-2,4-phenylene-cyclobutane (*poly*-bppcb) fused together with a 1D coordination polymer to furnish a MOF. The polymerization of 1,4-bis[2-(4’-pyridyl)ethenyl]benzene (bpeb) occurs inside a six-fold interpenetrated MOF with by [2+2] cycloaddition reaction of the slip-stacked packing of the adjacent bpeb ligands. This single-crystal-to-single-crystal (SCSC) structural transformation resulted in a MOPF (2), due to the formation of cyclobutane rings between the neighboring double bonds. Depolymerization occurs by the cleavage of cyclobutane rings in 2 to 1 in an SCSC manner when 2 was heated at 250 °C for 3 h. These highlight the advantages of solid state in the synthesis of highly crystalline metal complexes of organic polymers.



Slip-stacked packing of bpeb in MOF **1**
Showing the alignment of c=c bonds

poly-bppcb chain in MOPF **2**

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[발표취소] Containing chiral ligand aluminium complex for ROP of LA accompanying epimerization

고민정 강이영 이준승[*]

전남대학교 화학과

발 표 취 소

본 논문은 발표취소된 논문입니다.

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[발표취소] Fe(I)-Ru supramolecular M_4L_2 Cages From Tetrapyridyl Metalloligands

류지연 박유진 이준승*

전남대학교 화학과

발 표 취 소

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[발표취소] Zinc and Aluminum SALEN Complexes for Luminescent Polylactide

강이영 고민정 이준승* 박형련

전남대학교 화학과

발 표 취 소

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Synthesis and Hydrolysis of a 14-Membered Tetraaza Macrocycle Bearing *N*-Propargyl Pendant Arm and its Nickel(Ⅱ) Complex

김주영 강신걸*

대구대학교 화학과

A 14-membered tetraaza macrocycle 1,8-bis(propargyl)-5,5,7,12,12,14-hexamethyl-1,4,8,11-tetraaza (L^2) has been prepared by the reaction of 5,5,7,12,12,14-hexamethyl-1,4,8,11-tetraazacyclotetradecane(L^1) with propargyl bromide. The *cis*-octahedral nickel(Ⅱ) complex $[NiL^2(OAc)]^+$ as well as the square-planer complex $[NiL^2(OAc)]^+$ has been prepared and characterized. The *N*-propargyl pendant arms of $[NiL^2(OAc)]^+$undergoes hydrolysis in acidic and basic aqueous solutions to give various types of functionalized macrocyclic complexes. Interestingly, the reactions are strongly influenced by the pH of the reaction solutions. Synthesis and reaction solutions. Synthesis and reactions of L^2 and its nickel(Ⅱ) complexes are presented.

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Hydroamination of the *N*-$CH_2C{\equiv}CH$ Groups Attached to a Tetraaza Macrocyclic Nickel(Ⅱ) and Copper(Ⅱ) Complexes

이지영 강신걸* 곽지훈[1]

대구대학교 화학과 [1]순천대학교 화학교육과

The two *N*-$CH_2C{\equiv}CH$ pendant arms on the nickel(Ⅱ) complex $[NiL^2]^{2+}$ (L^2 = 2,13-bis(propargyl)-3,4-dimethyl-2,6,13,17-tetraazatricyclo[16.4.0.$^{1.18}$0$^{7.12}$]docosane) readily react with primary alkyl amine (RNH_2) to yield the octahedral complex $[NiL^3]^{2+}$ bearing two *N*-$CH_2C(=CH_2)NHR$ pendant arms that are involved in coordination. On the other hand, the copper(Ⅱ) $[CuL^2]^{2+}$ reacts with RNH_2 to give the square-pyramidal complex $[CuL^4]^{2+}$ bearing one *N*-$CH_2C{\equiv}CH$ and one *N*-$CH_2C(=CH_2)NHR$ pendant arms. The reaction of the complexes is strongly influenced by the nature of the central metal ion. The *N*-$CH_2C(=CH_2)NHR$ pendant arm(s) of $[NiL^3]^{2+}$ and $[CuL^4]^{2+}$ are not protonated even low pH. Synthesis and chemical properties of the functionalized macrocyclic complexes are presented.

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Reactions of Secondary Amines with *N*-Cyanometyhl groups Attached to a Macrocyclic Nikel(Ⅱ) Complex: Synthesis and Chemical Properties of Poly(macrocyclic) Nickel(Ⅱ) Complex

김현자 강신걸*

대구대학교 화학과

The N-CH_2CN groups attached to a tetraaza macrocyclic nickel(Ⅱ) complex react with various types of secondary amines, such as diethylamine and 14-membered tetraaza macrocycles. The reaction of $[NiL^1]^{2+}$(L^1+2,13-bis(cyanomethyl)-3,4-dimethyl-2,6,13,17-tetraazatricyclo[16.4.0.$^{1.18}$0$^{7.12}$]docosane) with R_2NH produces $[NiL^2]^{2+}$ bearing two coordinated *N*-$CH_2C(=N)NR_2$ pendant arms. In particular, $[NiL^1]^{2+}$(L^1 = 2,13-bis(cyanomethyl)-3,4-dimethyl-2,6,13,17-tetraazatricyclo[16.4.0.$^{1.18}$0$^{7.12}$]docosane) reacts with one of the secondary amino groups of 5,5,7,12,12,14-hexamethyl-1,4,8,11-teraazacylotetradecane (L^3) to yield the mononuclear tris(macrocyclic) complex $[NiL^4]^{2+}$ where the uncoordinated tetraaza macorcycles (L^2) are appended. In the presence of nickel(Ⅱ) ion, interestingly, $[NiL^4]^{2+}$ undergoes C-N bond cleavage, forming the mononuclear complexes $[NiL^1]^{2+}$ and $[NiL^3]^{2+}$. Synthesis, characterization, and chemical properties of the complexes are presented.

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Structure, Spectroscopy and Ligand Field Analysis of a Novel trans-anti-[Cr(Me2tn)2(N3)2]ClO4.2H2O

최종하* 이창섭[1] 유건상 홍용표

안동대학교 응용화학과 [1]계명대학교 화학과

trans-anti-[Cr(Me2tn)2(N3)2]ClO4.2H2O was prepared and its structure was determined by synchrotron radiation-based single-crystal X-ray diffraction at 95 K. The complex crystallized in the space group C2/c of the monoclinic system with four mononuclear formula units in a cell of dimensions a = 16.600 (3), b = 7.709 (2), c = 16.865 (3) Å, and β = 99.07 (3)°. The chromium ion was in a distorted octahedral coordination with four N atoms of two chelating Me2tn ligands and two N atoms of the azido group in the trans axial position. The two six-membered rings in the complex adopted only anti chair-chair conformations with respect to each other The important bond lengths are Cr-N(azide) 2.007 (2), Cr-N(Me2tn) 2.081 (2), 2.082 (2), N-N(azide) 1.184 (2) and 1.156 (2) Å, respectively. The ligand field analysis as well as the IR and electronic spectral properties are discussed.

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Synthesis, Crystal Structure and Ligand Field Properties of trans-Diaquahydroxobis(2,2-dimethyl-1,3-propanediamine)chromium(III) Diperchlorate

최종하* <u>이창섭</u>[1] 유건상 홍용표

안동대학교 응용화학과 [1]계명대학교 화학과

A novel complex trans-[Cr(Me2tn)2(OH)(H2O)](ClO4)2 was prepared and its structure was determined by single-crystal X-ray diffraction at 100 K. The complex crystallized in the space group P21/n of the monoclinic system with two mononuclear formula units in a cell of dimensions a = 5.980 (2), b = 8.312 (2), and c = 20.554 (4) Å. The chromium ion was in a distorted octahedral coordination with four N atoms of two chelating Me2tn and two O atoms of hydroxy group and water molecule in trans axial position. The two six-membered rings in the complex cation adopted anti chair-chair conformations with respect to each other. The mean Cr-N(Me2tn) and Cr-O bond lengths are 2.086 (2) and 1.907 (9) Å, respectively. The crystal lattice was stabilized by hydrogen bonding interactions among the oxygens of ClO4-, hydrogens of H2O and OH-, and NH groups of the Me2tn ligand. The IR and electronic spectral properties were discussed.

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발표분야: 무기화학

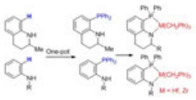
발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis of half metallocene complexes of phosphine-amido ligands for ethylene/α-olefin copolymerization

이춘선 이분열*

아주대학교 분자과학기술학과

2-R-(C9H9NH) (C9H10NH, tetrahydroquinoline) or N-R-C6H5NH was ortho-lithiated by the treatment of tBuLi after -NH group was converted to -N(COOLi). The ortho-lithiated compounds were reacted with Ph2P(OPh) to attach Ph2P-unit on the lithiated ortho-position. Reaction of the resulting compounds with M(CH2Ph)4 afforded a series of Hf and Zr complexes [(2-R-8-Ph2P-C9H9N)Hf(CH2Ph)3 (8, R=H; 9, R=Me; 10, R=iPr; 11, R=nBu), (N-R-2-Ph2P-C6H5N)Hf(CH2Ph)3 (12, R=Me; 13, R=Et; 14, R=iPr), [(2-R-8-Ph2P-C9H9N)Zr(CH2Ph)3 (15, R=H; 16, R=Me; 17, R=iPr; 18, R=nBu), (N-R-2-Ph2P-C6H5N)Zr(CH2Ph)3 (19, R=Me; 20, R=Et)]. The determination of the structures of 9, 14, 16, and 19 by x-ray crystallography reveal a distorted trigonal bipyramidal with two benzyls in equatorial position and the rest occupying an apical position, but the benzyl ligands scrambled, observing a single benzyl signal in the 1H NMR spectra. The complexes shows comparable activities (17-48?106 g/mol-M?h) in ethylene/1-octene copolymerizations to the CGC (36?106 g/mol-Ti?h). 15 showed exceptionally high 1-octene content (7.7 mol%) while the others showed low 1-octene contents (3-4 mol%). However, these 1-octent contents were significantly lower than that attained with the CGC (17 mol%). 9 and 16 generated high-molecular-weight polymers with Mw > 200000 even at a high temperature of 100-130 °C.


H
NH
Me
H
NH
R
One-pot
PPh$_2$
NH
Me
PPh$_2$
NH
R
Ph Ph
P
M(CH$_2$Ph)$_3$
N
R
Ph Ph
P
M(CH$_2$Ph)$_3$
N
R
M = Hf, Zr

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발표종류: 포스터, 발표일시: 수 16:00~19:00

Multi-Compositional Hybrid Coordination Polymer Particles (CPPs)

김현정 이희정 오문현*

연세대학교 화학과

The tuning of the chemical composition of nano-sized particles is an excellent way to regulate their properties. The construction and the characterization of well-organized homogeneously-compositional hybrid coordination polymers or metal-organic frameworks (MOFs) are remained as a critical challenge. Herein, the formation of well-structured hybrid coordination polymer particles (CPPs) is demonstrated via a solvothermal reaction. Furthermore, the compositions of the resulting hybrid CPPs are regulated by altering the amount of the starting building blocks.

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발표종류: 포스터, 발표일시: 수 16:00~19:00

Substitutent Effect of *o*-Carborane on the Photophysical Properties of Cyclometalated Ir(III) Complexes

박지현 김예진 이영훈[1] 이민형[*]

울산대학교 화학과 [1]울산대학교 기초과학연구소

A series of *o*-carborane substituted $(C^\wedge N)_2Ir(acac)$ complexes, $[4\text{-}(2\text{-}RCB)ppy]_2Ir(acac)$ (R = H, alkyl, aryl; CB = *o*-carboran-1-yl; acac = acetylacetonate) were prepared and characterized to investigate the 2-substituent effect of *o*-carborane on the photophysical properties of cyclometalated Ir(III) complexes. X-ray crystal structures of complexes were determined to see the variation of C_{cage}-C_{cage} bond distances and of torsion angles upon R substitution. UV/vis absorption and phosphorescence measurements under various conditions show that the photophysical properties in terms of quantum efficiencies and phosphorescence wavelength are dependent on the R substituent. Details of synthesis, characterization, and photophysical and electrochemical properties will be discussed.

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

A Fluorescence Sensor for Zn(II) and Al(III) and Colorimetric Sensor for Fe(II) and Fe(III)

최예원 이명미 이선영 김 철[1,*]

서울과학기술대학교 정밀화학과 [1]서울과학기술대학교 정밀화학과 친환경소재제품센터

A simple and easily synthesized fluorescent and colorimetric chemosensor 1, based on juloidine-imidazole moieties as a binding and signaling unit, has been synthesized in a one-step procedure. Receptor 1 showed immediate responses toward Zn^{2+} and Al^{3+} ions through selective fluorescence enhancement in buffer-acetonitrile and dimethylformamide (DMF) solution, respectively. Moreover, receptor 1 sensed the two states (Fe(II) and Fe(III)) of iron by “naked eye” with the different color. Upon the addition of Fe^{2+} and Fe^{3+} into each solution of 1, the color of the solutions instantly changed from colorless to orange for Fe^{2+} and to purple for Fe^{3+}. Thus, this sensor provides a novel approach for selectively recognizing the biologically important three elements in the human body simultaneously, for Zn^{2+} and Al^{3+} by emission spectra and Fe^{2+} and Fe^{3+} by the naked eye.

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발표종류: 포스터, 발표일시: 수 16:00~19:00

A new fluorescent sensor for sequential detection of zinc and copper ions

박경진 유가림 이명미 이재준 김 철[1,*]

서울과학기술대학교 정밀화학과 [1]서울과학기술대학교 정밀화학과 친환경소재제품센터

Sequential recognition of Zn^{2+} and Cu^{2+} by a new anthracene-containing dipyridylamine-based receptor 1 (N-((anthracen-9-yl)methyl)-N-(pyridin-2-yl)pyridin-2-amine) has been achieved. Receptor 1 exhibited highly selective and sensitive fluorescence “off-on” recognition property to Zn^{2+} with a 1:1 binding stoichiometry. The resulting 1-Zn^{2+} complex displayed high selectivity to Cu^{2+} through the decrease in fluorescence intensity, demonstrating that 1-Zn^{2+} could detect Cu^{2+} via metal displacement. The sequential recognition of Zn^{2+} and Cu^{2+} via metal exchange suggests that receptor 1 has a potential utility for Zn^{2+} and Cu^{2+} detection.

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발표종류: 포스터, 발표일시: 수 16:00~19:00

Selective Detection of Aluminum by Using Fluorescent and Colorimetric Methods in Aqueous Solution

이슬아 박경진 조현용 유가림 김 철[1,*]

서울과학기술대학교 정밀화학과 [1]서울과학기술대학교 정밀화학과 친환경소재제품센터

We have synthesized a new Schiff base 1, which detects Al^{3+} through fluorescence and naked eye in aqueous solution. The sensor 1 exhibited selective and sensitive recognition towards Al^{3+} via significant fluorescence enhancement (31-fold). Moreover, it showed a significant color change from colorless to yellow. The complex formation was proposed to be 1:1 ratio, based on Job plot, ESI-mass spectrometry analysis, ^{1}H NMR titration, and IR analysis. The detection limit was 1.00 μM, which is below the WHO acceptable limit (1.85 μM) in drinking water. In addition, the sensor 1 could be recyclable simply through treatment with a proper reagent such as EDTA.

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발표종류: 포스터, 발표일시: 수 16:00~19:00

Recognition of Zn^{2+} in 100% Aqueous Solution and F- in Organic Solvent

조현용 이슬아 최예원 김 철[1,*]

서울과학기술대학교 정밀화학과 [1]서울과학기술대학교 정밀화학과 친환경소재제품센터

A structurally simple 2-((1-hydroxynaphthalene-2-yl)methyleneamino)acetic acid (1) was used as a turn-on fluorescent sensor for bothZn^{2+} and F$^-$.This receptor 1 showed a significant fluorescence enhancement in the presence of zinc ion over most other competitive metal ions in 100% aqueous solution. In particular, this chemosensor could clearly distinguish Zn^{2+} from Cd^{2+}. The spectroscopic studies suggested that the selective response to zinc ion involved the disruption of the internal charge transfer (ICT), and the inhibition of the C=N isomerization and the excited-state proton transfer (ESIPT). In vitro studies with fibroblasts showed fluorescence when sensor 1 and Zn^{2+} were present. The receptor 1 could also sense F$^-$ selectively in DMSO. The fluorescence, UV-vis titration and 1H NMR titration indicated that F$^-$ ion enhanced the fluorescence of 1 through deprotonation.

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A highly selective fluorescent Zn(II) sensor based on quinoline

나유정 김용성 박대열 김 철[1,*]

서울과학기술대학교 정밀화학과 [1]서울과학기술대학교 정밀화학과 친환경소재제품센터

A quinoline-based simple receptor (bis(2-quinolinylmethyl)benzylamine = 1) as a Zn^{2+} selective fluorescent chemosensor showed a large fluorescent enhancement with a blue shift in the presence of Zn^{2+} which is attributed to a chelation enhanced fluorescence (CHEF) effect with inhibition of a photoinduced electron transfer (PET) process of 1. In particular, this receptor could clearly distinguish Zn^{2+} from Cd^{2+}. The binding mode of 1 and Zn^{2+} was found to be a 1:1 and confirmed by Job plot, ^{1}H NMR titration and ESI-mass spectrometry analysis.

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Solid-state synthesis, structure determination, and characterization of a new ternary scandium tellurite

이동우 옥강민*

중앙대학교 화학과

Pure bulk phase and single crystals of a novel ternary scandium tellurite, Sc2Te3O9 has been prepared through standard solid-state reactions using Sc2O3 and TeO2. The crystal structure of Sc2Te3O9 was determined by single-crystal X-ray diffraction. Sc2Te3O9 exhibits a three-dimensional framework structure consisting of distorted ScO6 octahedra, ScO7 capped octahedral, and TeO3 polyhedera. The Te4+ cations are in asymmetric coordination environment attributed to the stereoactive lone pairs. Thermal analysis reveals that the reported material is thermally stable up to 820 ?C. Infrared spectrum of Sc2Te3O9 shows characteristic bands for Sc?O and Te?O vibrations. UV-vis diffuse reflectance spectrum, elemental analysis, and dipole moment calculations are also presented.

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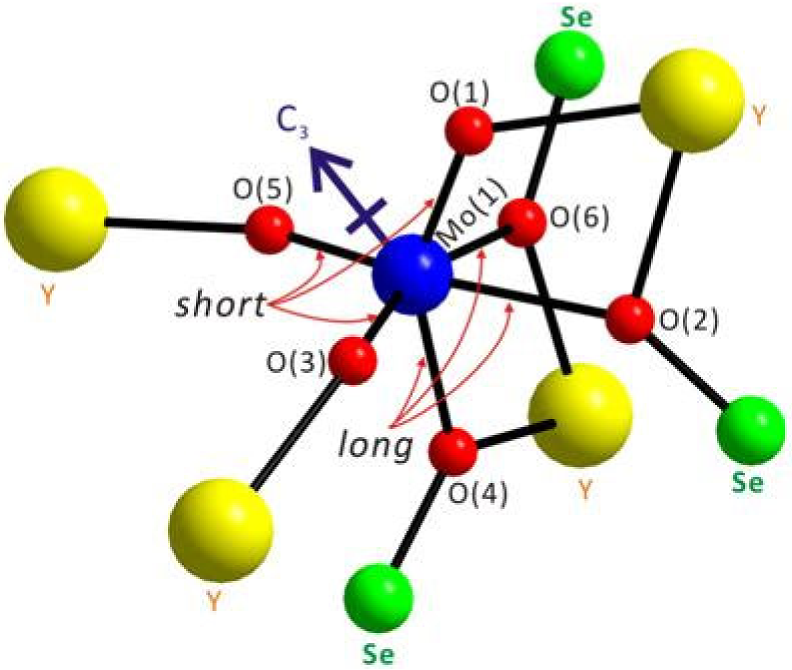
Effect of the lone pair cation, Se^{4+} on the out-of-center distortion of the d^0 cation, Mo^{6+}: synthesis, structure, and characterization of a new quaternary mixed metal oxide, $Y_2MoSe_3O_{12}$

방성은 옥강민*

중앙대학교 화학과

Noncentrosymmetric (NCS) compounds belong to a class of crystalline materials that is lacking an inversion center. NCS materials exhibit technologically important physical properties such as piezoelectricity, pyroelectricity, ferroelectircity and second-harmonic generations.[1] Second-order Jahn-Teller(SOJT) distortive cations are most often observed in two families of cations with asymmetric coordination environments, i.e., octahedrally coordinated d0 transition metals (Ti^{4+}, Nb^{5+}, W^{6+}, etc.) and lone pair cations (Sn^{2+}, Se^{4+}, Te^{4+}, etc.).[2]A new quaternary mixed metal oxide compound, $Y_2MoSe_3O_{12}$ containing both d0 transition metals (Y^{3+}, Mo^{6+}) and lone pair cation (Se^{2+}) has been prepared by a standard solid-state reaction using Y_2O_3, MoO_3 and SeO_2 as reagents. The structure of the reported material has been determined by single-crystal X-ray diffraction. Elemental analyses, infrared spectroscopy, thermal analyses and dipole moment calculations for the compounds are presented. An effect of the lone pair cation, Se^{4+} on the out-of-center distortion of the d0 cation, Mo^{6+} will be also discussed.


Se
O(1)
Y
C3
O(5)
Mo(1)
O(6)
Y
short
O(2)
O(3)
long
Y
Se
O(4)
Y
Se
Y
Se

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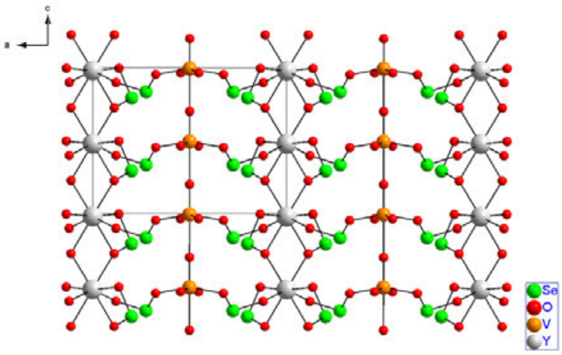
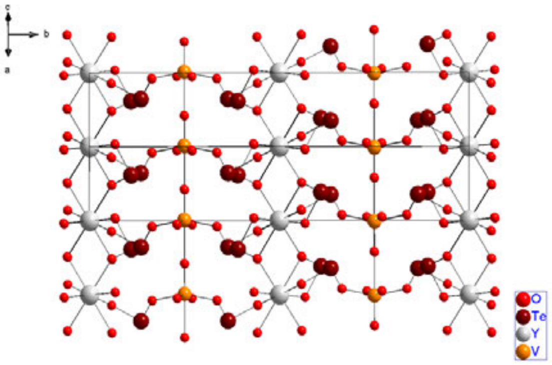
Effect of Lone Pair Cation Size on the Macroscopic Centricities in New Quaternary Yttrium Vanadium Selenite and Tellurite

김영훈 옥강민*

중앙대학교 화학과

Two new quaternary yttrium vanadium selenium/tellurium oxides, $YVSe_2O_8$ and $YVTe_2O_8$, have been synthesized by hydrothermal and standard solid-state reactions. Crystallographic analyses indicate that $YVSe_2O_8$ and $YVTe_2O_8$ have three-dimensional (3D) frameworks that are composed of layers of corner-shared VO_6 octahedra, layers of edge-shared YO_8, and SeO_3 or TeO_3 groups. Although stoichiometrically similar, $YVSe_2O_8$ crystallizes in the orthorhombic noncentrosymmetric (NCS) space group, *Abm*2, whereas $YVYe_2O_8$ crystallizes in the monoclinic centrosymmetric space group *C*2/m (No. 12). Since the average radii and the cation?lone pair distance for Te^{4+} are much greater than those for Se^{4+}, $YVTe_2O_8$ requires more space around YO_8 polyhedra and crystallizes in a CS space group. $YVSe_2O_8$ and $YVTe_2O_8$ are thermally stable up to 550 and 700 ^{O}C, respectively. Powder second-harmonic generation (SHG) measurements using 1064 nm radiation reveals that NCS $YVSe_2O_8$ has a SHG efficiency of 10 X α-SiO_2. The observed SHG response is attributable to a net dipole moment occurring along the [00-1] direction.





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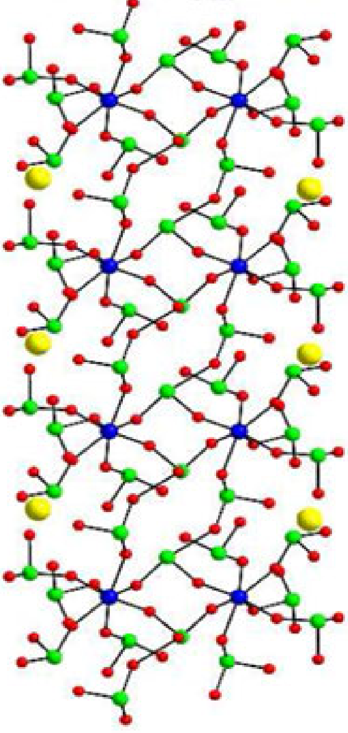
Infinite bands *vs*. isolated molecules : flexible coordination numbers of Zr^{4+} in new quaternary zirconium iodates materials

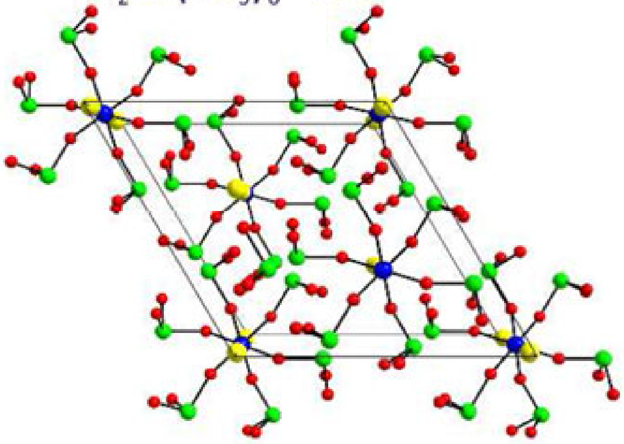
안현선 옥강민*

중앙대학교 화학과

Two new barium-and potassium-zirconium iodates, i.e., $BaZr(IO_3)_6$ and $K_2Zr(IO_3)_6$, have been synthesized through hydrothermal reactions using $BaCO_3$(or K_2CO_3), ZrO_2, and HIO_3 as reagents. Both single crystal and powder X-ray diffraction were used to determine crystal structures of the reported materials. While $BaZr(IO_3)_6$ exhibits an infinite band structure that consists of ZrO_7 pentagonal bipyramids and IO_3 trigonal pyramids, $K_2Zr(IO_3)_6$ reveals a zero-dimensional structure that is composed of ZrO_6 octahedra and IO_3 groups. The dimensionality variations are thought to be the effect of flexible coordination numbers of Zr^{4+} cations with large ionic radii. Also, the number of counter cations plays an important role to determine the dimensions of products. Both of the reported materials are thermally stable up to 440—450 °C. UV-vis diffuse reflectance spectra for $BaZr(IO_3)_6$ and $K_2Zr(IO_3)_6$ have been collected and absorption (*K/S*) data were calculated from the Kubelka-Munk function. Infrared spectra and local dipole moment calculations are also presented.



$BaZr(IO_3)_6$ - 1D



$K_2Zr(IO_3)_6$ - 0D

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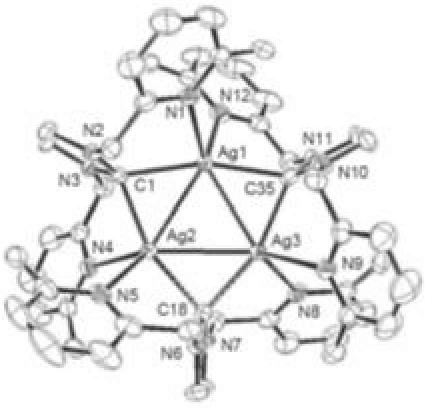
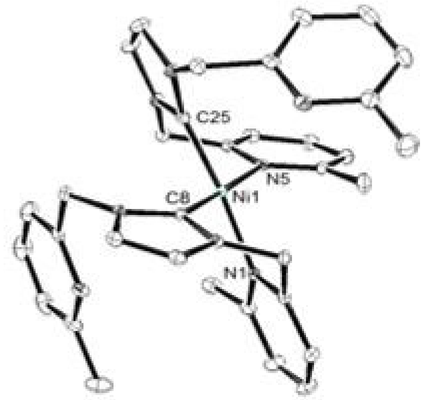
Formation of Ag(I) and Ni(II) N-heterocyclic Carbene Complexes: Synthesis, Characterization and Antimicrobial Activity Studies

정현진 임세리 박경세[1] 이동헌*

전북대학교 화학과 [1]군산대학교 화학과

N-heterocyclic carbene(NHCs) has steadily precedence over the most popular ligands in coordination chemistry due to their outstanding σ-donating properties, structural and theoretical studies and π-backbonding ability. For this reason, NHCs are diversely used as ancillary ligands to stabilize both main group and transition metals. Herein, the scope of our NHC ligand is extended by containing two pyridyl substituents $(MepyCH_2)_2$-Im, 1. Accordingly 1 make the metal complexes of the M_3L_3 or ML_2 types (metal-ligand) stoichiometry with Ag(I) and Ni(II) ions. By various analytical methods including X-ray crystallography, Ag(I) and Ni(II) complexes have been fully characterized. The silver complex, $[((MepyCH_2)_2\text{-Im})_3Ag_3](PF_6)_3$, 2, consists of distinct trinuclear silver ions. The Ni(II) complex of 1 is formulated as $[((MepyCH_2)_2\text{-Im})_2Ni](PF_6)_2$, 3 and a single-crystal X-ray structural determination confirms the formulation. The antimicrobial activities of these complexes were investigated against pathogenic bacteria for instance Staphylococcus aureus and it was shown that complex 2 exposed mild to moderate activity. Advanced for antibacterial agent, hydrolysis and bioassay studies are being planned.


N1
N12
N2
Ag1
N11
N3
C1
C35
N10
N4
Ag2
Ag3
N9
N5
C18
N8
N6
N7


C25
N5
C8
Ni1
N14

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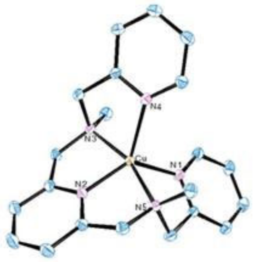
Synthesis, Characterization of Copper(II) and Zinc(II) Complexeswith Polypyridyl Chelates Ligand

정현진 문건우[1] 박경세[2] 이동헌*

전북대학교 화학과 [1]전북대학교 자연과학대학 화학과 [2]군산대학교 화학과

Many metal complexes with chelate pyridyl ligands in bioinorganic chemistry have received much attention in recent years because of their potential applications as functional materials, enzymatic reaction mechanism. Furthermore, copper and zinc compounds are one of the most frequently occurring element in the essential biochemical pathways. In this study, we have designed new pyridyl chelate ligand N,N'-(pyridine-2,6-diylbis(methylene))bis(N-methyl(pyridin-2-yl)methanamine) L^{N5} and synthesized it's metal complexes that $[Cu(L^{N5})](ClO_4)_2$ 1 and $[Z(L^{N5})](ClO_4)_2$ 2. The solid state structures of all two complexes were determined by single crystal X-ray diffraction studies. The Molecular structures of 1 and 2 Show a distorted square pyramidal geometry for the Zn(II) ion and Cu(II) ion. The UV-visible spectrum of 1 contain a single at 668 nm (ε=208 $M^{-1}cm^{-1}$) with an additional weak, broad and featureless absorption appearing at 948 nm (ε=119 $M^{-1}cm^{-1}$) in near- IR region. The X-band EPR spectrum of the 1 in solution revealed axial symmetry with $g_{\parallel}=2.04$ ($A_{\parallel}=148$ gauss), $g_{\perp}=2.24$ indicating an environment for Cu(II) ion with a $d_{x^2-y^2}$ ground state. The results are also proved that 1 has square pyramidal geometry in solution state. And We have studied electrochemical properties by using cyclic voltammetry. The cyclic voltammetric measurements indicated one-electon reversible reduction of the 1 occurring single quasi-reversible redox wave with $i_{pa}/i_{pc}=0.9\sim1.1$ at Ag/AgCl and corresponding 2 is irreversible process in this potential range. This research paper is in the field of coordination chemistry 5-coordinated metal complex on the expectation of a larger bioinorganic utilization.



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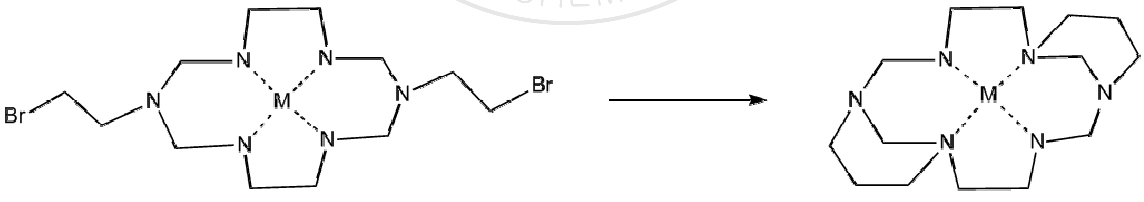
Preparation and further reaction of hexaazamacrocyclic complex having N-3-bromopropyl pendant arms

이재명 곽지훈[1,*]

순천대학교 화학과 [1]순천대학교 화학교육과

Polyazamacrocyclic complexes which contain functional side chains are interesting because not only the introduction of pendant arm into polyazamacrocyclic ligands makes the structural and chemical property of the complexes changed considerably but also the donor atoms in pendant arms of the complexes can be coordinated to another metal ions, resulting to self-assembled heterometallic complexes. We performed an attempted synthesis to get the hexaazamacrocyclic complex having N-bromopropyl pendant arms (1). However, we obtained the complex 2 having caged skeleton, which is the product from further reaction of 1. In this presentation, the preparation and characterization of 1 and 2 will be discussed in detail.



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2

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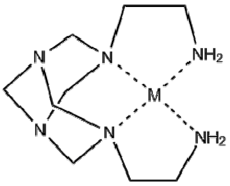
Synthesis and optical properties of the nickel(II) and copper(II) polyazamacrocyclic complexes combined with tetracyanoplaniate(II)

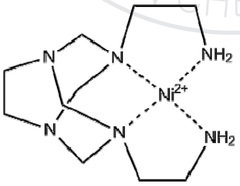
서민지 곽지훈[1,*]

순천대학교 화학과 [1]순천대학교 화학교육과

Preparation and application of EL material composed of metal-organic material is interesting because it has the thermal stability and it could be modified emission wavelength easily. Especially, lots of platinum complex has been applied to the EL material. Sometimes, this complex shows dramatic luminescent property in stacked solid derived from metal-metal interaction, which is normal property of noble metals. We prepared the supramolecules from the self-assembly of nickel(II) and copper(II) polyazacomplexes (1-4) and tetracyanoplatinate(II) and explored their optical properties. In this presentation the structure and emission properties of the supramolecules will be discussed in detail.



1 (M = Ni(II))
2 (M = Cu(II))



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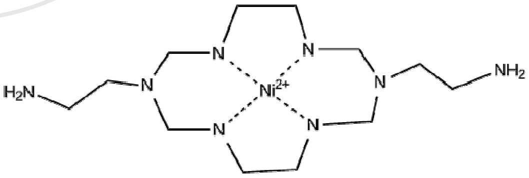

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Pd(II) complex with *N,N',X*-tridentate ligands (*X* = *N, O, S*) and their catalytic activity of methyl methacrylate polymerization

김성훈 이효선[1,*]

경북대학교 화학과 [1]경북대학교 자연과학대학 화학과

The reaction of [Pd(CH_3CN)$_2$$Cl_2$] with ancillary ligands, including *N*,*N*-dimethyl-3-((pyridin-2-ylmethylene)amino)propan-1-amine (L_1), 3-methoxy-N-(pyridin-2-ylmethylene)propan-1-amine (L_2), *N*-(3-(methylthio)propyl)-1-(pyridin-2-yl)methanimine (L_3), N,N-dimethyl-3-((quinolin-2-ylmethylene)amino)propan-1-amine (L_4), in the presence of $NaClO_4$, in ethanol yields [(*NN'X*)PdCl]ClO_4. The X-ray crystallographic analysis revealed that the palladium atoms of all complexes have a distorted square plane geometry involving three coordination atoms and a chloride ligand. All Pd(II) complexes were investigated for catalytic ability toward methyl methacrylate (MMA) polymerization.

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Synthesis, structure and characterisation methyl methacrylate polymerization of Cu(II), Co(II), and Cd(II) complexes with *N'*-cycloalky substituted *N,N*-bispyrazolyl ligands

최성혜 이효선[1,*]

경북대학교 화학과 [1]경북대학교 자연과학대학 화학과

New complexes [L_nMX_2] (L_n = L_1, L_2, M = Cu, Co, Cd, X = Cl, Br) was synthesized by the reaction of the corresponding metal starting materials with *N,N*-bis((1H-pyrazol-1-yl)methyl)cyclopentanamine (L_1) and *N,N*-bis((1H-pyrazol-1-yl)methyl)cyclohexanamine (L_2), respectively. The X-ray crystal structure of [L_1CuCl_2] is best described as a distorted tetrahedral geometry involving non-coordination of the nitrogen atom of the cycloalkyamine moiety and the Cu(II) center, resulting in the formation of an eight-membered chelate ring. However, [L_nCoCl_2] (L_n = L_1, L_2) and [L_2CdBr_2] complexes revealed that the cobalt atom in [L_nCoCl_2] (L_n = L_1, L_2) and cadmium in [L_2CdBr_2] showed distorted trigonal bipyramidal resulting from a coordination of the nitrogen atom of the cycloalkyamine moiety and the metal center. [L_nCoCl_2] (L_n = L_1, L_2) showed the highest catalytic activity for the polymerisation of methyl methacrylate (MMA) in the presence of modified methylaluminoxane (MMAO) among the others.

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N, N-di (2-picolyl) cyclohexylamine coordinated to the transition metals of Cu(II), Cd(II) and Zn(II) complexes: Synthesis, characterization and methyl methacrylate polymerization

송유진 이효선[1,*]

경북대학교 화학과 [1]경북대학교 자연과학대학 화학과

A new series of $[(dpca)M(II)X_2]$ (M = Cu, Cd, Zn and X = Cl, Br, NO_3) complexes were synthesized by the reaction of *N,N*-di(2-picolyl)cyclohexylamine (dpca) with corresponding metal starting materials. X-ray crystallographic analysis determined that the metal centre in complexes, $[(dpca)CuCl_2]$, $[(dpca)CdBr_2]$ and $[(dpca)Zn(NO_3)_2]$ showed significantly distorted 5-coordinated trigonal bipyramidal geometry involving a coordination of the nitrogen atom of cyclohexylamine moiety and the metal centre. Specifically, the catalytic activity of $[(dpca)Zn(NO_3)_2$ in the polymerization of methyl methacrylate (MMA) in the presence of modified methylaluminoxane (MMAO) at 60°C were higher than that of $[(dpca)CdBr_2]$ and $[(dpca)CuCl_2]$.

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Synthesis of copper complexes bearing naphthalenylmethyl derivatives of (*R*,*R*)-1,2-diaminocyclohexane and their application to *rac*-Lactide polymerization

조재원 정종화*

경북대학교 화학과

Two novel dichloro copper complexes of *N*^{1},*N*^{2}-dimethyl-*N*^{1},*N*^{2}-bis(naphthalen-2- ylmethyl)cyclohexane-1,2-diamine ligands were synthesised and characterised by X-ray diffraction. The alkoxide derivatives of the well characterized dichloro copper(II) complexes were assessed for ring opening polymerization (ROP) of *rac*-Lactide. The active catalyst species were generated by treating the copper complexes with 2 equivalent $LiOCHMe_2$. Furthermore, the heterotactic polylactide with P_r up to 83 % can be obtained by using the initiator of the complex bearing *N*^{1},*N*^{2}-dimethyl-*N*^{1},*N*^{2}-bis(2-naphthalen-2-ylmethyl)cyclohexane-1,2-diamine in CH_2Cl_2 at -25℃. The stereoselectivity and molecular weight of the polymer was determined by ^{1}H-NMR spectra, and GPC.

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Cu(II) complexes containing *N,N'*-bidentate *N'*-Substituted *N,N*-iminopyridines: The formation of monomeric versus dimeeric species

김성훈 안승현 이효선[1,*]

경북대학교 화학과 [1]경북대학교 자연과학대학 화학과

The reaction of [$CuCl_2$] and *N,N'*-bidentate 1-(furan-2-yl)-N-(pyridin-2-ylmethylene)methanamine (L_1) and 2-(piperidin-1-yl)-N-(pyridin-2-ylmethylene)ethanamine (L_2) in ethanol yields monomeric [L_1CuCl_2] and dimeric [$L_2Cu(u\text{-}Cl)Cl]_2$ complexes, respectively. The X-ray crystal structure of [L_1CuCl_2] and [$L_2Cu(u\text{-}Cl)Cl]_2$ revealed that the copper atom in [L_1CuCl_2] and [$L_2Cu(u\text{-}Cl)Cl]_2$ were 4-coordinated distorted tetrahedral and 5-coordinated distorted trigonal-bipyramidal geometry, respectively.

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Size Dependent Photocatalytic Activity of Fe3O4@HP Magnetic Particles

김운호 이규동[1] 정진승[1,*]

강릉원주대학교 화학신소재 [1]강릉원주대학교 화학과

Porous magnetite submicron particles were fabricated successfully using a solvothermal method. The size control of Fe3O4 particles has been adjusted by controlling the rate of VEG/VDEG.We developed multifunctional Fe3O4@HP particles functionalized by coating them with hematoporphyrin(HP) for introducing a photo-functionality.Microstructure and magnetic properties of the photofunctional magnetic nanoparticles are investigated by TEM, SEM, and VSM. Photocatalytic experiment of the Fe3O4@HP particles (2,4,6-TCP) solutions illuminated under Xe light in a photochemical reactor.

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Copolymerizations of 2,5-Dibromo-1,1-diethyl-3,4-diphenylsilole wiht Dichlorodisubstitutedsilanes or Dichlorotetrametyldisilane and their Properties

장지훈 박영태[1,*]

계명대학교 화학과 [1]계명대학교 자연과학대학 화학과

2,5-Dibromo-1,1-diethyl-3,4-diphenylsilole as monomers were prepared by the intramolecular reductive cyclizations of diethyl bis(phenylethynyl)silane with treatments of 4 mol lithium naphthalenide followed by anhydrous $ZnCl_2$ and N-bromosuccinimide in situ. We have synthesized new polymeric materials of polycarbosilanes containing 1,1-diethyl-3,4-diphenyl-2,5-silole and disubstitutedsilanes or dichlorotetramethyldisilane along the polymer main chain by copolymerizations of 2,5-dibromo-1,1-diethyl-3,4-diphenylsilole with several dichlorodisubstitutedsilane or dichlorotetramethyldisilane using n-butyllithium. The obtained polycarbosilanes are soluble in usual organic solvents such as THF and $CHCl_3$. The prepared materials were characterized by GPC, ^1H, ^{13}C, NMR, and IR spectroscopies along with TGA. We also studied the electronic properties of the prepared polycarbosilanes by UV-vis absorption, excitation and fluorescence emission spectroscopic methods, in particular.

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

정영민 박영태[1,*]

계명대학교 화학과 [1]계명대학교 자연과학대학 화학과

2,5-Dibromo-1,1-diisopropyl-3,4-diphenylsilole as monomer was prepared by the intramolecular reductive cyclization of diisopropylbis(phenylethynyl)silane with treatment of 4 mol lithium naphthalenide followed by anhydrous $ZnCl_2$ and N-bromosuccinimide in situ. We have synthesized new polymeric materials of polycarbosilanes containing 1,1-diisopropyl-3,4-diphenyl-2,5-silole and disubstitutedsilane along the polymer main chain by copolymerizations of 2,5-dibromo-1,1-diisopropyl-3,4-diphenylsilole with several dichlorodisubstitutedsilane using n-butyllithium. The obtained polycarbosilanes are soluble in usual organic solvents such as THF and $CHCl_3$. The prepared materials were characterized by GPC, NMR, and IR spectroscopies along with TGA. We also studied the electronic properties of the prepared polycarbosilanes by UV-vis absorption, excitation and fluorescence emission spectroscopic methods, in particular. Also, through electrical characteristics and property evaluation research, we will apply these polymeric binder to a secondary battery by mixing a secondary battery binder with conductive material. In order to improve conductivity and adhesive property.

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Synthesis of Polydimethylsiloxane-graft-Polyethyleneoxide by Hydrosilation and their properties

정영민 박영태[1,*] 장지훈 민용기 오소영[2]

계명대학교 화학과 [1]계명대학교 자연과학대학 화학과 [2]계명대학교 규소화학/화학과

Polydimethylsiloxane-graft-Polyethyleneoxide have been studied for cosmetic and personal care formulations. These polymers have highly functional unique properties such as surface active property and applicability. These properties are attributed to tendency of the silicone polyethyleneoxide copolymers to orient at the interface between two compatible phases. To improve wetting behavior as well as foam characteristics, these copolymers are used to reduce the surface tension of aqueous formulation.The general structure of silicone polymer has water repellent property which is hydrophobic, but it doesn't have hydrophilic portion. So it is necessary to be introduced into the polymer chain of silicone materials. We have synthesized Polydimethylsiloxane-graft-Polyethyleneoxide by hydrosilations of H-Silicon oil with allyl-ethyleneoxide using platinum catalyst without solvents. The prepared silicone polyethyleneoxide copolymers were characterized by gel permeation chromatography (GPC), ^{1}H, ^{13}C, ^{29}Si NMR, FTIR and elemental analysis, etc.

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Tuned CO_2 sorption properties of isoreticular and polymorphic Metal-Organic Frameworks by combinational synthetic approaches

정석 나명수*

울산과학기술대학교(UNIST) 화학과

Isoreticular and polymorphic 3-D pillared metal-organic frameworks (MOFs) prepared via combinational synthetic approaches such as direct solvothermal reactions, postsynthetic ligand exchanges of the MOFs prepared via the direct solvothermal reactions, and postsynthetic ligand insertions show outstanding CO_2working capture capacity. The pore properties, including the pore dimensions and geometries and the specific surface areas of a series of MOFs prepared via the combinational synthetic approaches, were investigated. The potentials of the MOFs as postcombustion CO_2 capture materials based on the working CO_2 capture capacities in vacuum swing adsorption and pressure swing adsorption processes are discussed.

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Isoreticular metal-organic frameworks based on quadruply interlinked a rhombic dodecahedral metal-organic polyhedron as a tertiary building unit

김동욱 나명수*

울산과학기술대학교(UNIST) 화학과

The solvothermal reactions of a Zn(II) ion and two tetracarboxylate ligands with different flexibility, respectively, lead to the isoreticular metal?organic frameworks (MOFs), PMOF-4 and PMOF-5, based on a rhombic dodecahedral metal?organic polyhedron (MOP) as a 24-c tertiary building unit (TBU). The rhombic dodecahedral MOP was composed by six dinuclear Zn square paddle wheel clusters, $[Zn_2(COO)_4]$ as a 4-c secondary building unit (SBU) and eight dinuclear Zn trigonal paddle wheel clusters, $[Zn_2(COO)_3]$ as a 3-c SBU. The network of the isoreticular MOFs as a 3,3,4-c net with a zjz topology was distinguishable from the similar MOFs, PMOF-3 and PCN-12, with 24-c cuboctahedral Cu-MOP as another type of TBU. However, both 24-c TBUs in all MOFs were quadruply interlinked to six neighboring TBUs to form the networks of the same pcu underlying topology.

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Study on spin crossover behavior of iron(III) complexe with NNO type ligands: crystal structure and magnetic property

정아림 안승현 민길식[1,*]

경북대학교 화학과 [1]경북대학교 사범대학 화학교육과

Spin crossover (SCO) compounds have been recived much attentions because of their potential and/or practical applications for data storage devices, molecular switches, displays and sensors. In our group, new iron(III) spin crossover complex, $[(3,5\text{-Cl-qsal})_2\text{Fe}](NO_3)\cdot H_2O$ (1), has been prepared by the Fe(III) species with 3,5-dichloro-*N*-(8-quinolyl)salicylamine (3,5-Cl-qsal) in an aerobic condition. The structure of 1 was determined by single crystal X-ray diffraction at 100 and 298 K, respectively. In 1, an iron(III) ion was coordinated with two 3,5-Cl-qsal ligands shown six-coordinate distorted octahedral geometry with an N_4O_2 donor set. At 100 and 298 K, the average Fe-N/O distances are 1.915(1) and 2.040(1) Å and relate to low spin and high spin states, respectively. 1 displays spin crossover behaviors about 230 K with approximately 10 K width of the thermal hysteresis loop. In this poster, we will present the detailed preparation of the ligand and iron compound, crystal structure, magnetic properties as well as interesting coordination chemistry.

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Nanoparticulate Hollow Co3O4 Oxidation Catalysts from Hollow Microporous Organic Networks

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Various microporous organic networks (MONs) have been prepared through various carbon-carbon coupling reactions between organic building blocks. The porosity and functionalities of MONs could be controlled by using predesigned building blocks. The resultant materials have been applied for gas adsorbents and catalysts. In addition to inner porosity, the overall shape of porous materials is also important for their performances. To interact with inner working sites in adsorption or catalysis, guest molecules should diffuse into pore structures. The diffusion pathways are dependant on the shape of materials and can be synthetically engineered. For example, hollow inorganic spheres showed better efficiencies in electrochemical or photocatalytic performances than non-hollow ones. By using silica templates, monodisperse hollow MONs were synthesized through the chemical etching after the coupling reaction. In addition to inorganic templates, organic ones have been developed and used for the shape controlled synthesis of inorganic materials because they can be easily removed through heat treatment under air condition. In this research, the hollow MONs were served as an organic template for nanoparticulate Co3O4 hollow spheres. The resultant Co3O4 showed excellent catalytic activities in H2O2 oxidation for the removal of organic pollutants in water through the reaction of resultant radical (·OH) species.

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Synthesis, X-ray crystal structure, and methyl methacrylate polymerisation of binuclear cobalt(II) and cadmium(II) complexes with tetradentate pyrazolyl ligands

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The reaction of anhydrous [$CoBr_2$] and [$CdBr_2(H_2O)_4$] with ancillary ligands, including 4,4'-oxybis-(*N*,*N*-bis-(1H-pyrazolyl-1-yl)methyl)aniline) (L_1) and 4,4'-methylenebis-(*N*,*N*-bis((1H-pyrazolyl-1-yl))methyl)aniline (L_2), respectively, in ethanol yields [$L_nCo_2Br_4$] (L_n = L_1 and L_2) and [$L_2Cd_2Br_4$] complexes. The X-ray crystal structures of complexes revealed that they are binuclear, and each metal atom has a distorted tetrahedral geometry which involves a nitrogen atom from two pyrazole groups and two chloro ligands. The catalytic activity of [$L_nCo_2Br_4$] (L_n = L_1 and L_2) and [$L_2Cd_2Br_4$] for the polymerisation of methyl methacrylate (MMA) in the presence of modified methylaluminoxane (MMAO) was compared to the corresponding binuclear zinc complex [$L_2Zn_2Cl_4$].

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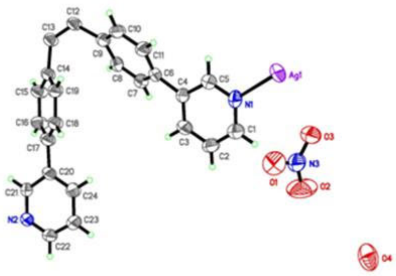
Silver coordination polymers constructed by a C4-symmetric tetrapyridyl ligand and silver halides: {[Ag2(L)]?(NO3)2?(H2O)2}∞, {[Ag(L)]?(PF6)}∞, {[Ag2I2L](CH2Cl2)}∞, {L = tetra((3-pyridyl)phenyl)ethylene {(3-py)-4-Ph}2C=C(Ph-4-(3-py)2}

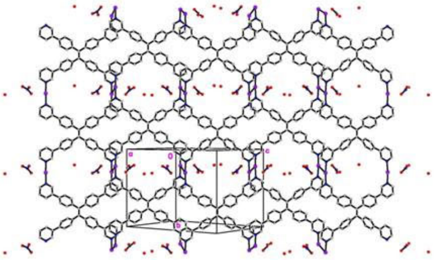
이강민* 이순원*

성균관대학교 화학과

Three coordination polymers, {[Ag2(L)]?(NO3)2?(H2O)2}∞ (1), {[Ag(L)]?(PF6)}∞ (2), and {[Ag2I2L](CH2Cl2)} ∞(3) [L= 1,1,2,2-tetrakis(4-(pyridin-3-yl)phenyl)ethene], were prepared under solvent diffusion method.The structure of polymer (1) is a 2-D. However {[Ag(L)]?(PF6)}∞ (2), and{[Ag2I2L](CH2Cl2)} ∞(3) were 3-D polymers. When the counterion is I?,it acts as aligand to form an I- bridged Ag4I4 core and participate in the two repeat units, which are connected to a three-dimensional framework.Keywords: solvent diffusion, counter ion, bridging ligand.

Polymer 1





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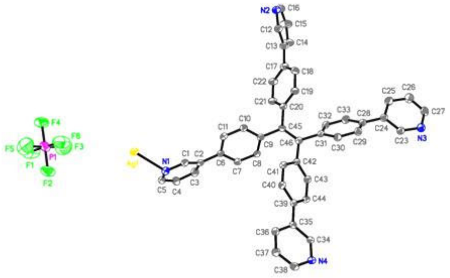
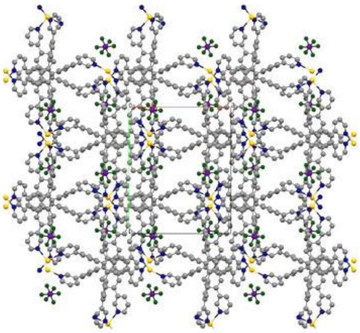
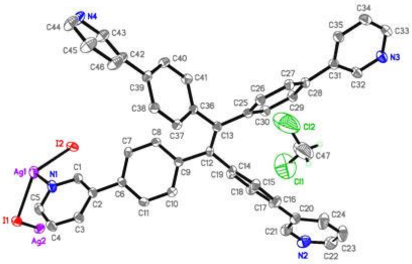
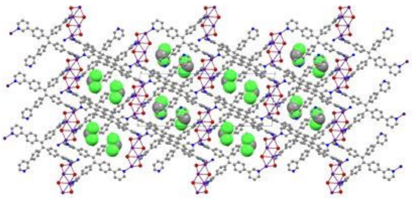




Polymer 3





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Self-assembly and characterization of 2-D metal-organic framework from nickel(II) macrocyclic complex with pentyl groups and *cis,cis*-1,3,5-cyclohexanetricarboxylic acid

박지혜 정아림[1] 민길식[2,*]

경북대학교 화학교육 [1]경북대학교 화학과 [2]경북대학교 사범대학 화학교육과

The nickel(II) hexaaza macrocyclic complex (1) containing pendent pentyl groups has been synthesized by the one-pot template condensation reaction of amines and formaldehyde. From the self-assembly of 1 with deprotonated *cis,cis*-1,3,5-cyclohexanetricarboxylic acid, CTC^{3-}, 2-D supramolecular network of $[Ni(C_{18}H_{42}N_6)]_3[C_6H_9(COO)_3]_2?6CH_3CN?6H_2O$ (2) has been constructed. The solid 2 is insoluble in any solvents and violet in the solid state. The X-ray crystal structure of 2 indicates that each nickel(II) macrocyclic unit binds two CTC^{3-} ions in trans position, and each CTC^{3-} ion coordinates three nickel(II) macrocyclic complexes which are extended to form a 2-D layer. In this poster, we will present the detailed preparation and structure of 1 and 2 as well as physical properties.

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Steric effects on the reactivity of Ni-O_2 complexes toward organic substrates

이준형 박예훈 조재홍*

대구경북과학기술원(DGIST) 신물질과학

Mononuclear metal-O_2(M-O_2) adducts are implicated as key intermediates in dioxygen activation reactions in biology. Thus, the study of structure, spectroscopic properties, and reactivity of biomimetic models of M-O_2 is essential in synthetic inorganic chemistry. Herein, we report the preparation of different type of pyridinophane ligands: N,N′-di-tert-butyl-2,11-diaza[3.3](2,6)pyridinophane (TBDAP) and N,N′-cyclohexyl-2,11-diaza[3.3](2,6)pyridinophane (CHDAP) in order to investigate the steric effect on the reactivity of Ni-O_2 complexes toward external substrates. These ligands were characterized by ^{1}H-, ^{13}C-NMR and ESI-MS. The Ni(III)-O_2 complexes containing pyridinophane type ligands were successfully generated and characterized with various physicochemical methods. The reactivity of Ni(III)-O_2 species bearing CHDAP toward organic substrates is higher than that of Ni(III)-O_2 species bearing TBDAP.

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New type of π - extented Porphyrin dimers : Application in Organic Photovoltaic Cells

박우재 이석중*

고려대학교 화학과

In recent years, studies of soluble π-conjugated porphyrins have produced considerably interesting results for their applications in organic optoelectronic devices, such as the organic photovoltaic cells (OPVCs) for alternate energy sources. OPVCs using small band gap molecules with different repeating units for the modulation of the optical band gap have been studied. Porphyrin dimers as strong π?conjugated molecules have been intensively studied because of their importance in the fields of photochemical, photobiological, and photovoltaic applications. They exhibit efficient electron transfer, and highly photosensitive properties with the structure of a large and planar π-conjugation. In order to improve the optical absorption properties, new functionalized dimer derivatives with controlled two porphyrin units and a π-conjugated configuration can be suggested. We synthesized porphyrin dimers, and fabricated OPVCs composed of these porphyrin dimer as a donor with PCBM as an acceptor.

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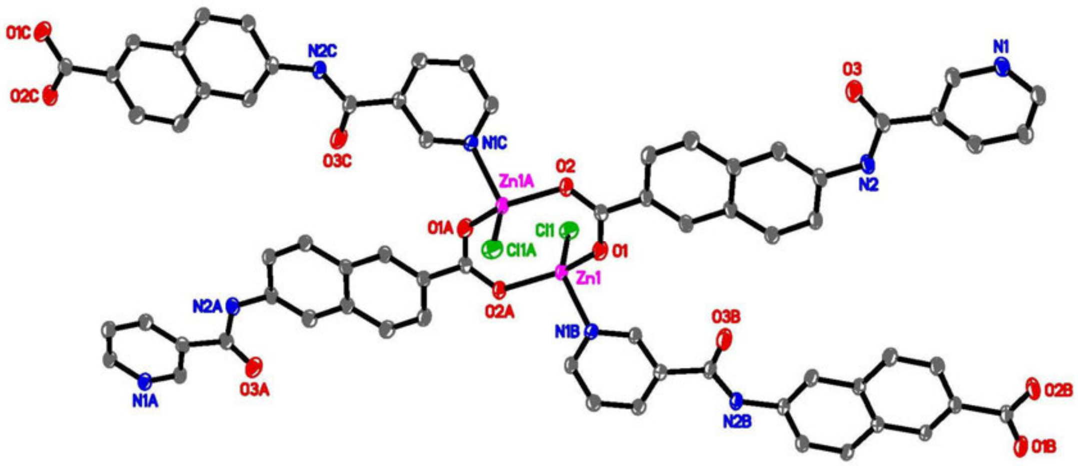
A Two-dimensional Zn Coordination Polymer Based on a Pyridyl-Carboxylate Linking Ligand Containing an Intervening Amide Group: $[ZnCl(L)]_\infty$(HL = 6-(nicotinamido)-2-naphthoic acid)

박수진* 이순원*

성균관대학교 화학과

Zinc complex, [ZnCl(L)] {L = [(3-py)-C(O)=N(H)-$C_{10}H_6$-COO^-]}, was prepared from zinc chloride, 6-(nicotinamido)-2-naphthoic acid {HL = [(3-py)-C(O)=N(H)-$C_{10}H_6$-COOH]}, and 1M NaOH in H_2O under hydrothermal conditions. The local coordination environment of the Zn^{2+} ion in polymer is given in Figure below, in which two Zn^{2+} ions are joined by a bridging carboxylate group. The Zn^{2+} ion is coordinated to one nitrogen and two oxygen atoms from three ligands. The amide group does not coordinate to the metal. The amide N-H bond forms a weak intermolecular hydrogen bond with the Cl ligand. The structure of product was determined by X-ray diffraction.



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Unidirectional Photo-induced Charge Separation and Thermal Charge Recombination of Cofacially Aligned Donor-Acceptor System Probed by Ultrafast Visible-Pump/Mid-IR-Probe Spectroscopy

노희창 강윤경*

상명대학교 화학과

New pi-stacked donor-acceptor (D-A) systems, [Ru(1-([2,2'-bipyridine]-6-yl-methyl)-3-(2-cyclohexa-2’,5’-diene-1,4-dionyl)-1H-imidazole)(2,2’:6’,2”-terpyridine)]$[PF_6]_2$ (ImQ_T) and [Ru(1-[2,2’-bipyridine]-6-yl)-3-(2-cyclohexa-2’,5’-diene-1,4-dionyl)phenyl)(2,2’:6’,2”-terpyridine)]$[PF_6]_2$ (PhQ_T), have been synthesized and characterized. Similar to their precedent, [Ru(6-(2-cyclohexa-2’,5’-diene-1,4-dione)-2,2’:6’,2”-terpyridine)(2,2’:6’,2”-terpyridine)]$[PF_6]_2$ (TQ_T), these systems have a cofacial alignments of terpyridine (tpy) ligand and quinonyl (Q) group, which facilitate electron transfer through pi-stacked manifold. Despite the presence of lowest-energy charge transfer transition from the Ru-based-HOMO-to-Q-based-LUMO (MQCT) predicted by theoretical calculations by using time-dependent density functional theory (TD-DFT), the experimental steady-state absorption spectra do not exhibit such bands. The selective excitations to the Ru-based occupied orbitals-to-tpy-based virtual orbital MLCT states were thus possible, from which charge separation (CS) reactions occurred. The photo-induced CS and thermal charge recombination (CR) reactions were probed by using ultrafast visible-pump/mid-IR-probe (TrIR) spectroscopic method. Analysis of decay kinetics of Q and Q- state CO stretching modes as well as aromatic C=C stretching mode of tpy ligand gave time constants of

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Prediction of Redox Potential Inversion of Series Ruthenium Aqua Complexes by DFT Calculation

김문주 강윤경*

상명대학교 화학과

Llobet and coworkers has reported a design strategy of Ru complexes for the efficient water oxidation (*J. Am. Chem. Soc.* 2006, *128*, 5306) based on the early study of Dovletoglou and Meyer (*Inorg. Chem.* 1996, *35*, 4120). Their work has shed some light on the design motives of water-splitting catalyst in terms of the selection of ligand systems of the Ru complexes. Here we present a method that forecast a redox potential inversion of any given Ru-aqua complex, a situation where the second oxidation potential is more favorable thermodynamically than the first. We have explored electron transfer energetics of several Ru complexes reported by Dovletoglou and Meyer by using density functional theory to reproduce the experimentally determined oxidation potentials. Calculation results of systematic variations of exchange-correlation functionals as well as basis sets will be displayed.

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Synthesis and structural studies of cobalt complexes of N,N,N',N'-tetra-[(3,5-dimethyl-1-pyrazolyl)methyl]-2,2'-(ethylenedioxy)bis(ethylamine)(T-DPEE)

임종완

심인고등학교 화학

Two cobalt(III) complexes $[Co_2(T\text{-}DPEE)Cl_4]$, $[Co(D\text{-}DPEE)](BPh_4)_2$[D-DPEE=N,N'-di-[(3,5-dimethyl-1-pyrazolyl)methyl]-2,2'-(ethylenedioxy)bis(ethylamine)] and cobalt cubane complex have been prepared and characterized by X-ray diffraction measurements. T-DPEE having two pyrazole groups which were bridged by 2,2'-(ethylenedioxy)bis(ethylamine) so afford large chelating spatial for the formation of polynuclear complex. Dinuclear Co(II) complex was formed in the reaction of $CoCl_2 \cdot 6H_2O$ with T-DPEE. The crystallographic analysis of the complex revealed that the two N of pyrazole, one N of amine and two Cl atoms are bound to Co with trigonal bipyramidal geometry. In constrast to $CoCl_2 \cdot 6H_2O$ the reaction of $Co(OAc)_2 \cdot 6H_2O$ with pyrazole ligand formed Co_4N_4 Cubane Cluster.

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Control of luminescence properties in naphthalene- diimide-based gel with azobenzoic acid by charge transfer interaction with self-sorting effect

이지하 정종화*

경상대학교 화학과

An effective supramolecular strategy for preparation of a photoluminescent hydrogel with self-sorting between naphthalene-diimide as electron acceptor and diazobenzoic acid as electron donor is reported. This concept is based on the charge-transfer interaction between the donor and acceptor chromophores so that self-sorting ensured synergistic effects of π-stacking and charge-transfer interactions.

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SiO_2 나노입자를 이용한 Hg^{2+} 센서의 제조와 형광특성 연구

이진혁 정종화*

경상대학교 화학과

본 연구는 Hg^{2+} 이온을 검출하기 위해서 리간드 1 을 졸-젤공법에 의해서 나노입자표면에 도입하여 유기-무기 하이브리드 소재(S1)를 제조 하였다. 유기-무기 하이브리드 나노소재(S1)은 FT-IR, TGA 및 형광분광기를 이용하여 특성을 연구하였다. 그 결과 리간드 1 은 나노입자 표면에 공유결합에 의해서 20.8% 정도 도입되었다. 특히 수용액에 분산된 S1 은 360 nm 의 빛을 흡수한 결과 500 nm 에서 강한 방출 스펙트럼을 나타내었다. 따라서 수용액에 분산된 S1 의 형광특성은 다양한 금속이온(Cu^{2+}, Cd^{2+}, Na^{2+}, Zn^{2+}, Ag^{2+}, Pb^{2+}, Mg^{2+}, Hg^{2+})를 첨가하여 연구하였다. 그 결과 S1 의 형광특성은 Zn 이온을 첨가시 크게 증가하였으나, 다른 금속이온 (Cu^{2+}, Cd^{2+}, Na^{2+}, Ag^{2+}, Pb^{2+}, Mg^{2+}, Hg^{2+})의 경우에는 큰 변화가 나타나지 않았다. 이는 S1 에 도입된 리간드가 Zn^{2+} 이온과 선택적으로 결합하기 때문으로 예측된다.

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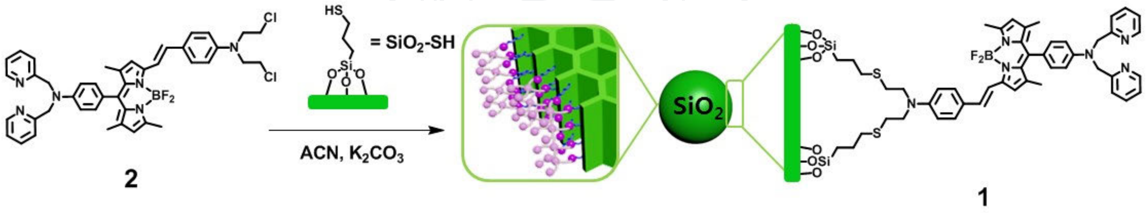
Fluorometric/colorimetric logic gates based on BODIPY-functionalized silica nanoparticles

최희경 이지하 정종화*

경상대학교 화학과

Functionalized nanoparticles are useful as colorimetric and fluorometric logic gates, which with various inputs such as metal ions induce photoinduced electron transfer (PET) and internal charge transfer (ICT) processes of functionalized nanoparticles. We have demonstrated that metal ions acting as modulators in BODIPY-functionalized SiO_2 nanoparticles can generate absorbance changes in accordance with the operation of a half-adder digital circuit. In addition, a NAND logic gate in the emission mode was obtained which exploited a different binding affinity for metal ions for different ligands.



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Concentration Programmed Helix Inversion of the Terpyridine-Based Supramolecular Gel Triggered by an Achiral Co^{2+} Ion

박소현 안준호 정성호 정종화*

경상대학교 화학과

The inversion and transfer of chirality information of supramolecular helices are ubiquitous phenomena in nature. Biological DNA and protein often alter their helix sense in response to particular external stimuli and switch biologically important events on. For example, the left-handed DNA, Z-DNA, is derived from a right-handed helix by salt enrichment, cytoshine methylation, and complexation with spermine, spermidine, and metal cations. we have demonstrated the formation of opposite helicities in co-existence of two different complexes from one enantiomer of a chiral ligand. The helicites of Co^{2+} complexes are strongly dependent to the concentration of Co^{2+}. **L1** containing S-form alanine moiety forms the octahederal structure of 1:2 complex at less than 0.5 equivalent of Co^{2+}, which has the M form with left helicity. In presence of 0.6 to 0.9 equivalent of Co^{2+}, two different of the octahedral and the square pyramidal structures of gels **L1** exist, which is dependent to Co^{2+} concentration. On the other hand, in 1.0 equivalent of Co^{2+}, **L1** forms the square pyramidal structure of 1:1 complex with Co^{2+}, which has the P form with right-handed helicity. In contrast, **L2** containing R-form alanine moiety complex with Co^{2+} exhibited an opposite helix inversion mechanism. Note that the helical inversion described herein differs from the inversion observed in supramolecular assemblies in sol state and also from the inversion of helicity observed in polymer systems. Co^{2+} complexes have been useful as highly stereoselective catalysts, effective building-block cores for molecular architecture, specific redox devices, and ion sensor.

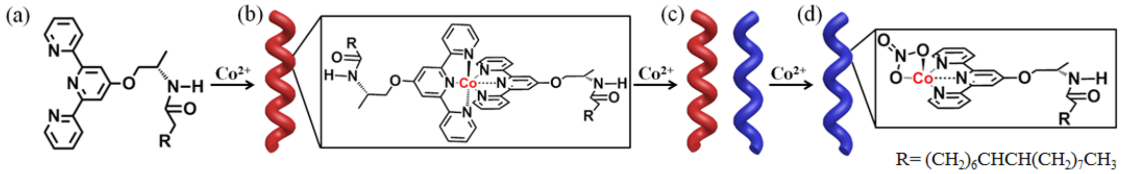

Fig. 1 structure of **L1**(a) in several equivalents of Co^{2+}. (b)0.1~0.5, (c)0.6~0.9, and (d)1.0 equivalent of Co^{2+}. Red and blue colored tubes indicate left-handed and right-handed helical structures, respectively.

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발표종류: 포스터, 발표일시: 수 16:00~19:00

Tetraphenylethylene의 AIE효과를 이용한 히스티딘 검출

김가영 정종화* 정성호

경상대학교 화학과

응집으로 형광이 유도되는(AIE ; Aggregation-Induced emission) 유기 발광단은 고체상태의 높은 양자효율로 인해 발광 재료, 센서 등의 연구에서 각광받고 있다. 본 연구에서는 그 중 대표적으로 AIE 효과를 나타내는 Tetraphenylethylene 을 기반으로 한 유도체(TIE **1** : 1,1,2,2-tetrakis(4-(1H-imidazol-1-yl)phenyl)ethene)를 제조하여 Cu^{2+}와 함께 화학적 센서 연구를 진행하였다. AIE 효과로 인한 **1** 이 형광이 나타나는 MeOH/H2O 조건에서 Cu^{2+}를 첨가하여 형광을 감소시켰다. 제조된 용액은 다양한 아미노산 첨가를 통해 관찰된 결과 히스티딘에서만 강한 형과을 나타내는 것을 볼 수 있었다. 이러한 결과는 **1** 에 배위되어 있던 Cu 가 2 당량의 히스티딘과 결합하여 다시 **1** 의 AIE 효과가 나타난 것으로 추측된다. 이로 인해 본 발표에서느 Cu^{2+}-**1** 용액의 히스티딘 검출 센서로서의 기능을 보여주고자 한다.

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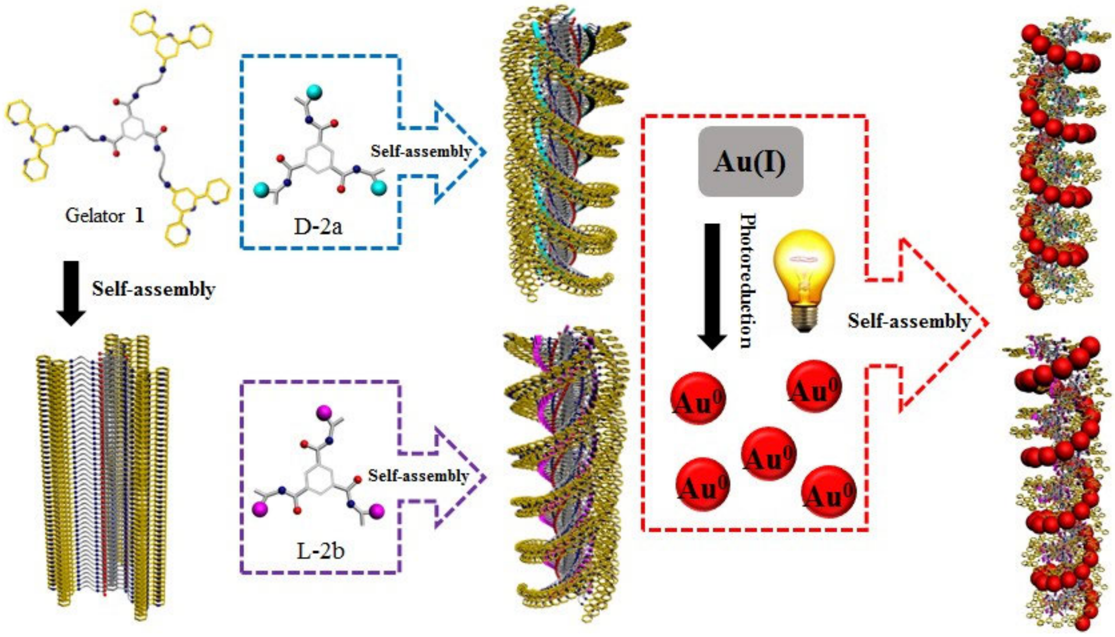
Chiral Arrangement of Achiral Au Nanoparticles by Supramolecular Assembly of Helical Nanofiber Templates

정성호 정종화*

경상대학교 화학과

Chiral materials comprised of organized nanoparticle superstructures have promising applications to photonics and sensing; however, reliable customization of the chiroptical properties of these materials has yet to be realized. In this work, Our approach to chiroptical materials development may help to extend the length scales of organized gold nanoparticles on helical nanofibers up to hundreds of nanometers in length with tunable nanoparticles diameters ranging from 2 nm up to 200 nm. The size of the gold nanoparticles comprising the superstructures could be easily controlled by UV irradiation time to facilitate flexibility in terms of the desired plasmon absorption wavelength. Moreover, we provide the first modular system in which the chiroptical properties of the hydrogels can be easily customized by addition of D-from (2a) or L-form (2b) helical introducing molecules to yield materials exhibiting a positive first Cotton effect and negative first Cotton effect, respectively. Utilizing this modular template in combination with controlled nanoparticle growth can offer high yield and predictable “bottom-up” assembly which we expect to be of significant value to researchers requiring materials with customizable chiroptical properties.


Gelator 1
Self-assembly
D-2a
Self-assembly
L-2b
Self-assembly
Au(I)
Photoreduction
Au0
Au0
Au0
Au0
Au0
Self-assembly

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발표종류: 포스터, 발표일시: 수 16:00~19:00

Luminescent Calix[4]arene-Based Metallogel Formed at Different Solvent Composition

박재현 이지하 정종화*

경상대학교 화학과

We have synthesized a calix[4]arene derivative (1) containing terpyridine and showed that gelation occurred in the presence of Pt^{2+} in DMSO/H_2O of varying composition. Gelation was presumably mediated by the Pt-Pt and π-π stacking interactions. SEM image of the xerogel showed a spherical structure with 1.8-2.1 μm of diameter. Interestingly, the metallogel showed strong luminescence enhancement, which depended on the DMSO/H_2O ratio of the solvent. We examined the effects of concentration, temperature, and time resolution on the luminescence emission of both the gel 1-Pt^{2+} and the sol 1-Pt^{2+}. The luminescence lifetimes of the metallogel were particularly very long, the order of several microseconds. The luminescence lifetimes were also strongly dependent on the solvent composition. We also determined the thermodynamic parameters in the formation of self-assembly of the gel, a quantitative treatment of the system based on the Birks scheme. Furthermore, the rheological properties of the metallogels in the presence of more than 4.0 equivalent of Pt^{2+} were independent of the concentration of Pt^{2+} application

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Radial Directional Charge Transport by Using Rod Type TiO_2 Electrode with PbS Colloidal Quantum Dot

이성희 김상욱[1,*]

아주대학교 분자과학기술학과 [1]아주대학교 응용생명화학공학부

To improve the performance of all-solid-state inorganic CQD sensitized solar cells (SSCs) , structure of Titanium dioxide(TiO_2) electrode which is 1D TiO_2 nanorod was regulated. New aligned PbS CQD-SSCs with radial directional chare transport system have efficiently reduced recombination due to shorter pathway. Also, pore space of 1D structured TiO_2 electrode can be more efficiently filled up with PbS quantum dot than mesoporous structured TiO_2. The device performance with 1D nanorod(NR) TiO_2 electrode showed R_s of 87.4 Ω, R_{sh} of 23.7 kΩ, FF 60.3 %. Those values were improved in comparison to mesoscopic nanoparticle based solar cells.

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Effect of extended aromatic ligand on photoactivated NO-releasing of Ruthenium Nitrosyl complexes

조장훈 이홍인*

경북대학교 화학과

Nitric oxide plays important roles in a wide variety of physiological processes, including neurotransmission, immune response, blood pressure control, and inhibition of tumor growth. For the purpose of controlling the physiological processes, compounds that selectively release nitric oxide have attracted considerable interest. Among them, nitrosyl ruthenium complexes have been proposed as attractive photodynamic therapeutic agents in biomedicine and in tumor treatment. This research aims at developing nitrosyl ruthenium complexes which absorb long wavelength visible light to release NO with high quantum yield. Previously, we have synthesized a series of [Ru(R-EBPP)(Cl)(NO)], where EBPP(=N,N'-(ethane-1,2-diyldi-o-phenylene)-bis(pyridine-2-carboxamide) has an electron-donating or withdrawing group R(=H, CH_3, OCH_3) for investigating their photoreactivities. The quantum yield values of the three cpmplexes follow the trend R =CH_3> H ~ OCH_3. To further improve the photoreactivity of the nitrosyl ruthenium complexes, we now developed the extension of conjugation in the ligand frame because the position of the photoband of the $\{Ru\text{-}NO\}^6$nitrosyl can be adjusted via substitution, extension of conjugation of the pyridine arms. The extension was performed by replacing the pyridine rings with quinolines. Both 1-isoquinoline (1-IQ) and 3-isoqulinoline (3-IQ) were used in the design of the ligand frames to isolate [(1-IQ)Ru(NO)(Cl)] and [(3-IQ)Ru(NO)(Cl)]. We present here other evidences of photoactivated NO-releasing and other properties monitored by UV-VIS, EPR and X-ray crystallography.

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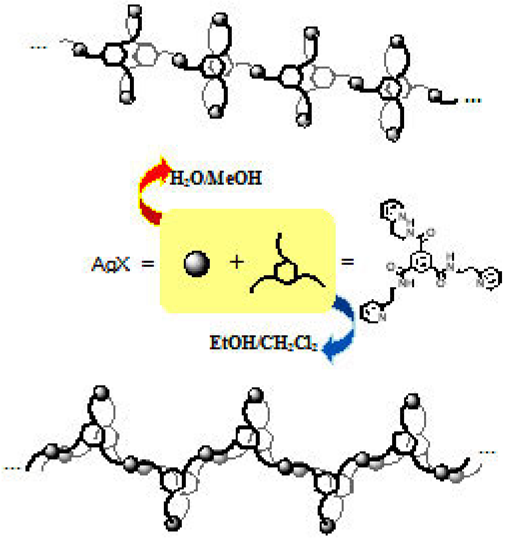
Investigation into Solvent Effects on Structure and the Related Physicochemical Properties of Silver(I) Coordination Polymers Containing *N,N',N"*-Tris(2-pyridinylethyl)-1,3,5-benzenetricarboxamide

<u>김은이</u> 정옥상*

부산대학교 화학과

Self-assembly of AgX ($X^{?}$ = $ClO_4^{?}$, $PF_6^{?}$) with *N*,*N'*,*N"*-tris(2-pyridinylethyl)-1,3,5-benzenetricarboxamide (L) in water and methanol solution yields $[Ag_3L_2](ClO_4)_3$ and $[Ag_3L_2](PF_6)_3?H_2O$, respectively, which are 1D coordination polymers of alternating cyclic moieties and linkage moieties. In contrast, the reaction in ethanol and dichloromethane solution produces unique zigzag-type molecular ladder structures of $[Ag_6L_4(H_2O)](ClO_4)_6?CH_2Cl_2?6H_2O$ and $[Ag_3L_2](PF_6)_3?2CH_2Cl_2?H_2O$, respectively. Solide-state PL spectra of the present complexes were observed at 455-466 nm. Their structural and physicochemical properties such as anion exchangeability, thermal behavior, and photoluminescence have been carefully investigated.


H$_2$O/MeOH
AgX =
+
=
EtOH/CH$_2$Cl$_2$

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Unprecedented Conglomerate Crystals of Discrete Palladium(II) Metallacyclophanes

이해리 정옥상*

부산대학교 화학과

The present study employed a self-assembly approach incorporating the above-noted three methods in order to construct racemic helical metallacyclophanes, (*P*,*M*)-$[Pd_3X_6(L_1)_2]$, via the reaction of K_2PdX_4 (X = Cl, Br) with the C_3-symmetric tridentate L_1 ligand as a programmed discrete helical component. Consecutive partial-substitution reaction of (*P*,*M*)-$[Pd_3X_6(L_1)_2]$ with another C_3-symmetric tridentate L_2 ligand, or direct self-assembly of K_2PdX_4 with both L_1 and L_2, produces unprecedented conglomerate crystals forming a ball-joint-type host-guest system, (*P*)-$[Pd_3X_6(L_1)_2]$@(*M*)-$[Pd_3X_6(L_1)(L_2)]$ and (*M*)-$[Pd_3X_6\ (L_1)_2]$@(*P*)-$[Pd_3X_6(L_1)(L_2)]$ (X = Cl, Br; L_1 = *N,N',N"*-tris(2-pyridinylethyl)-1,3,5-benzenetricarboxamide; L_2 = *N,N',N"*-tris(3-pyridinylpropyl)-1,3,5-benzenetricarboxylate; *P* = right-handed helix; *M* = left-handed helix). This host-guest system, significantly, represents an effective method of obtaining useful aggregates. We report herein a uniquely effective strategy for the synthesis of such a system. Its crystal structures, the driving aggregative force behind it, and the reversible equilibrium between the aggregate and its dissociated species in solution are also discussed.

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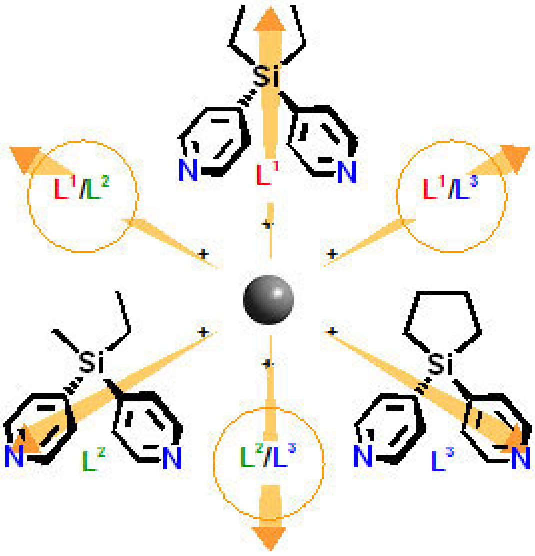
Investigations into Pure Bidentate Ligands vs Mixed Bidentate Ligands on Self-Assembly with Silver(I) Hexafluorophosphate

박민우 정옥상*

부산대학교 화학과

Investigations into pure bidentate ligands vs mixed bidentate ligands on self-assembly of $AgPF_6$ with the respective L^1, L^2, L^3, L^1/L^2, L^1/L^3, and L^2/L^3 (L^1 = diethylbis(4-pyridyl)silane; L^2 = ethylmethylbis(4-pyridyl)silane; L^3=cyclotetramethylenebis(4-pyridyl)silane) were carried out. The reactions of $AgPF_6$ with the respective ligand system produce desirable homoleptic or heteroleptic silver(I) coordination polymers. $[Ag(L^1)_2](PF_6)$ gives rise to a tubular loop chain whereas the other five products lead to a two-fold interpenetration diamonoid structure. $[Ag(L^1)_2](PF_6)$ shows a strong blue luminescence at 453 nm (λ_{ex} = 270 nm), which is useful to recognize alcohols. All products were characterized by thermal analyses, and in particular, calcination of $[Ag(L^3)_2](PF_6)$?CH_3OH at 600 ºC finally produces silver(0) microcrystalline morphology.



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발표분야: 무기화학
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Subtle Anion Effects on Construction and Photoluminescence of 1D Sinusoidal Zinc(II) Complexes

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부산대학교 화학과

Self-assembly of ZnX_2 (X = Cl, Br, and I) with a bidentate *N*-donor ligand, 2,7-bis(isonicotinoyloxy)naphthalene (L), yields 1-D sinusoidal chain of zinc(II) complexes, $[ZnCl_2(L)]\cdot 2CH_2Cl_2$, $[ZnBr_2(L)]\cdot 2CH_2Cl_2$, and $[ZnI_2(L)]\cdot CH_2Cl_2\cdot H_2O$, respectively. π-π interactions between naphthalene and pyridyl groups result in the formation of 1-D suprachannels occupied with each solvate molecule. Emission spectra of the present complexes were observed at 353-360 nm. For $[ZnCl_2(L)]\cdot 2CH_2Cl_2$, the significant PL enhancement was induced by the addition of p-hydroquinone. Calcination of the compounds produced zinc(II) oxide with the different morphologies checked by SEM images and EDX results.

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Photoluminescence and Catalytic Properties of Discrete Trimetallic Zinc(II) Complexes

장재성 이해리 정옥상*

부산대학교 화학과

Self-assembly of ZnX_2 (X = Cl, Br, and I) with C_3-symmetric tridentate N-donor ligand, *N,N',N"*-tris(2-pyridinylethyl)-1,3,5-benzenetricarboxamide (L), yields discrete trimetallic zinc(II) complexes, $[Zn_3X_6L(MeOH)_3]$. These form, via inter- and intra-molecular interactions, an ensemble constituting a columnar stacking structure in *abab*... staggered fashion. For this series of complexes, the halogen effects on the photoluminescence, catalysis, and thermal properties were investigated. For $[Zn_3Cl_6L(MeOH)_3]$, a blue luminescence was observed at 462 nm (λ_{ex} = 369 nm). The transesterification catalysis showed significant halogen effects in the order $[Zn_3I_6L(MeOH)_3] > [Zn_3Cl_6L(MeOH)_3] > [Zn_3Br_6L(MeOH)_3]$ in methanol, whereas in a mixture of methanol and acetonitrile, the order was $[Zn_3I_6L(MeOH)_3] > [Zn_3Cl_6L(MeOH)_3] > [Zn_3Br_6L(MeOH)_3]$. Such notable different effects among the three complexes might be explained by the halogens' electronic effects and dissociation properties. This catalysis work reveals that both direct halogen effects and solvent systems play significant roles in transesterification. Calcination of the materials results in formation of different morphologies of zinc(II) oxide. More systematic studies, for example on the synthesis of related ligands, are in progress. Further experiments, moreover, will provide more detailed information on the enormous potentials of the complexes' catalytic properties and photoluminescence.

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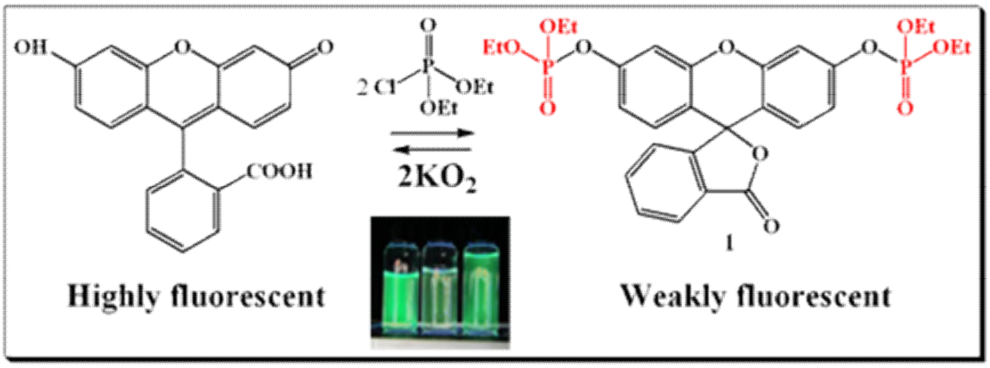
Novel reversible and selective nerve agent simulant detection in conjunction with superoxide “turn?on” probing

장윤정 **D.G.Churchill***

한국과학기술원(KAIST) 화학과

Chemical warfare agents (CWAs) are toxic chemicals used as offensive weapons of war. Among them, nerve agent are the most toxic and dangerous chemicals. Nerve agents interfere with cholinesterases (AChE) in nervous system and inhibit the AChE by phosphorylation and phosphonylation of Serine OH and make enzyme inactive. Inhibited AChE is not capable to hydrolyse the acetylcholine, thus it accumulates in synapses.1 Current methods to detect nerve agents include mass spectrometry, ion-mobility spectrometry, enzyme sensors, and chemical sensors.2 Detecting nerve agents using chemical sensors is the simplest and the most convenient way since it relies upon optical detection and cheap and easy to use. Fluorescein, which is a well-known fluorophore, was used as a reversible fluorescent probe for nerve agent simulant “ON?OFF” detection and subsequent superoxide detection. DCP (Diethyl chlorophosphate), DEMP (diethyl methylphosphonate) and DECP (Diethyl cyanophosphonate) were used as nerve agent simulants. Fluorescein can detect the nerve agent simulant DCP to give a fluorescent “on-off” signal. Additionally, superoxide allows for the regeneration of fluorescein from the phosphorylated fluorescein in an “off-on” method. The order of decrease in fluorescence intensity for nerve agents simulants is DCP > DEMP >> DECP.1. W. Wu, J. Dong, X. Wang, J. Li, S. Sui, G. Chen, J. Liu and M. Zhang, Analyst., 2012, 137, 3224. 2. (a) G. R. Asbury, C. Wu, W. F. Siems, and H. H. Hill Jr., Anal. Chim. Acta, 2000, 404, 273. (b) T. H. Henderson, Anal. Chem., 2002, 74, 191. (c) R. M. Black, R. T. Clarke, R. W. Read, M. J. J. Reid, J. Chromatogr. A, 1994, 662, 301. (d) A. Mulchandani, S. Pand, and W. Chen, Biotechnol. Prog., 1999, 15, 130.


OH
O
O
COOH
Highly fluorescent
2 Cl
P
O
OEt
OEt
2KO$_2$
EtO
OEt
P
O
O
O
O
OEt
OEt
P
O
O
1
Weakly fluorescent

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Synthesis, Crystal Structures, and Photoluminescent Properties of Silver(I) Complexes Bearing 2,3-Bis(isonicotinoyloxy)naphthalene

김정균 정옥상*

부산대학교 화학과

Investigations into the anion effects on formation and photoluminescence (PL) of a series of AgX (X^- = NO_2^-, NO_3^-, ClO_4^-, and PF_6^-) compounds with 2,3-bis(isonicotinoyloxy)naphthalene (L) were carried out. According to single crystal X-ray diffraction, NO_2^-, NO_3^-, and ClO_4^- anions act as anionic ligands rather than simple counteranions whereas PF_6^- anion acts as a simple counteranion. In particular, the dinitroargentate anionic species, $Ag(NO_2)_2^-$, was observed in the solid state for the first time. The PL intensity of the present compounds is proportional to the Ag…X distance, namely the metallophilicity of the anions. Weak- or non-coordinating anions, ClO_4^- and PF_6^-, could be smoothly exchanged to NO_2^- or NO_3^- anions while the reverse exchanges did not conducted. Their physicochemical properties were fully characterized by means of IR, TGA/DSC, and PL.

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Arabidopsis thaliana **SPL14전사인자에 결합가능한 DNA가 도입된 금 나노입자들을 이용한 자기조립 및 단백질 검출**

안준호 정성호 정종화*

경상대학교 화학과

본 연구는 말단에 싸이올 기를 지니는 상보적 두 DNA 를 각 금 나노입자 표면에 salt aging 방법으로 도입하여 연구를 수행 하였다. 상보적 염기서열을 지니는 DNA 가 도입된 두 종류의 금 나노입자는 혼합 함에 따라 DNA 간 수소결합에 의해 입자간 응집을 일으키며 변색되는 것을 UV-Vis 분광기, 임도분포 측정기, 투과전자현미경을 통하여 분석하였다. 이중나선을 형성한 채 응집된 금 나노입자의 결합 안정성 분석은 용액의 온도변화 및 염 농도 변화에 대한 UV-Vis 분광기를 측정하여 밝힐 수 있었다. 또한 SPL14 및 RPA 단백질의 첨가를 통해 이중나선을 형성한 채 응집된 두 입자의 결합 특성변화를 UV-Vis 분광기, 입도분포측정기, 투과전자현미경을 통하여 분석하였다. 이를 통해 DNA 가 도입된 금 나노입자가 SPL14 단백질의 특정 부분에 선택적 결합을 이루는 염기서열이 포함된 DNA 이중나선을 이룬 채 응집되어도 DNA 이중나선이 SPL14 전사인자에 작용한다는 것을 규명할 수 있었다.

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발표종류: 포스터, 발표일시: 수 16:00~19:00

Transition Metal Complexes with N,N'-(ethylene-di-p-phenylene)bis (pyridine-2-carboxamide) Ligand

김유정 이홍인*

경북대학교 화학과

Carboxamide group, found in the primary structure of proteins, is an important ligand construction unit for coordination chemistry. Phenyl-pyridyl-carboxamides, a growing class of multidentate ligands containing this linkage, are available from condensation reactions between pyridyl-bearing carboxylic acids and phenylamine precursors, promoted by a coupling agent such as triphenylphosphite. Metal complexes with phenyl-pyridyl-carboxamides have been found to be useful in asymmetric catalysis, molecular receptors and dendrimer synthesis. We have developed a tetradentate ligand, H_2EBPP (= N,N'-(ethylene-di-p-phenylene)bis(pyridine-2-carboxyamide)), to be utilized for synthesizing chromium, iron, nickel, copper, and ruthenium complexes. Structural charaterizations of the complexes revealed very intriguing coordination behaviors and metal oxidation states depending on metals. In this study, we present the syntheses, structures, and physical properties.

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Synthesis and Characterization of Dinuclear Copper Complex and its Catalytic Activity on the Oxidation of Catechol

홍수경 이홍인*

경북대학교 화학과

The work in this meeting presents the synthesis, characterization and catecholase activity, study of dinuclear copper(II) complex (Cu_2L_2) derived from a tetradentate dicarboxamide ligand H_2L (H_2L = *N*,*N'*-(Ethane-1,2-diyldi-*o*-phenylene)-bis(pyridine-2-carboxamide), obtained on (2:1) condensation of pyridine-2-carboxylic acid and 2,2'-ethylenedianiline. Single crystal X-ray crystallography of Cu_2L_2 showed that the two copper centers are apart at 6.992 ? , allowing this non-coupled dicopper(II) complex to be a model for the active sites of catechol oxidase. However, in the presence of Cu_2L_2, 3,5-di-tert-butylcatechol (3,5-DTBC) undergoes catalytic oxidative dehydrogenation to the corresponding 3,5-di-tert-butyl-*o*-benzoquinone (3,5-DTBQ) at room temperature and atmospheric dioxygen pressure. The semiquinone anion radical 3,5-di-tert-butyl-*o*-benzosemiquinone (3,5-DTBSQ$^{\cdot}$) and 3,5-di-tert-butyl-*o*-benzoquinone copper complex Cu_2L_2(3,5-DTBQ) have been detected as intermediate by ESR and ESI-MS. The catalytic activities were followed in methanol solvent and monitored by the UV-VIS and EPR spectroscopy.

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Synthesis of zinc oxide nanotubes and their application in dye-sensitized solar cells

임다혜 김진권[1,*]

공주대학교 화학과&GETRC [1]공주대학교 화학과

Nanostructured zinc oxide (ZnO) an exceptionally important semiconductor materials to study due to its attractive physical properties such as wide band gap (3.37 eV) and large exciton binding energy (60 meV) at room temperature. Because of its unique optical and electrical properties it has potential applications in UV lasers , light-emitting diodes (LED) , field-effect transistors solar cells and sensorsZnO nanotubes were synthesized through a combination of templating and solvothermal processes using Selenium nanowires as templates .These nanotubes were characterized by scanning electron microscopy (SEM), X-ray diffraction (XRD), transmission electron microscopy (TEM). The influence of ZnO nanotubes on the performance of dye-sensitized solar cells (DSSCs) based on the ZnO nanotube/nanoparticle composite films was investigated.

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Two dimensional dysprosium(Ⅲ) complex exhibiting field-induced slow magnetic relaxation

송정화 임광수 홍창섭*

고려대학교 화학과

We have synthesized a two-dimensional flexible coordination polymer $[Dy(p\text{-}XBP4)_{2.5}(H_2O)_3(CH_3OH)_3]\cdot W(CN)_8\cdot CH_3OH$ (1) (p-XBP4: N,N’-p-phenylenedimethylenebis(pyridin-4-one)) using a slow evaporation reaction of Dy(Ⅲ) nitrate, $Cs_3[W(CN)_8]$ and flexible ligand p-XBP4 in water/methanol mixed solvent. Compound 1 crystallizes in the triclinic system with the space group P-1 and consists of a $W(CN)^{3-}$ anionic part and a $[Dy(p\text{-}XBP4)_{2.5}(H_2O)_3(CH_3OH)_3]^{3+}$ cationic one. Each Dy^{3+} ion is coordinated by five oxygen atoms from p-XBP4 ligand and two oxygen atoms from water. Compound 1 was characterized by elemental analysis, IR, PXRD and single crystal X-ray diffraction. Detailed structural and magnetic studies will be given in the presentation.

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Synthesis, structural characterization, and magnetic properties of a 2-D dysprosium(III) system

임광수 홍창섭*

고려대학교 화학과

The reaction of dysprosium(III) nitrate, isophthalic acid, and the zwitterrionic dicarboxylate ligand 1,4-bis(4-carboxylatopyridinium-1-methylene)benzene (L) yielded a Dy(III) coordination polymer [Dy(isophtalate)(L)$_{0.5}$(isonicotinate)$_{0.5}$(formate)$_{0.5}$]·x(H_2O) (1·xH_2O) with carboxylate bridges. Complex 1 was characterized by elemental analysis, TG analysis, and single crystal X-ray diffraction. There are two crystallographically independent Dy(III) atoms in 1. Both Dy(III) ions adopt capped cube geometry and the local symmetry is close to C_{4V}. In the absence of dc field, the complex 1 shows weak frequency-dependent out-of-phase (χm”) signals of ac magnetic susceptibilities. This is due to the fast relaxation of the magnetization through a quantum tunneling process. In this presentation, detailed structures and magnetic properties will be discussed.

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발표종류: 포스터, 발표일시: 수 16:00~19:00

pH-Dependent Proton-Conducting Behavior in a Metal-Organic Framework Material

방원주 이우람 홍창섭*

고려대학교 화학과

A porous metal-organic framework (MOF) [Ni_2(dobdc)(H_2O)2]?6H_2O (Ni_2(dobdc) or Ni-MOF-74; dobdc^{4-} = 2,5-dioxido-1,4-benzenedicarboxylate) with hexagonal channels, was synthesized using a microwave-assisted solvothermal reaction. Soaking Ni_2(dobdc) in sulfuric acid solutions at different pH values afforded new proton-conducting frameworks, $H^+(H_2O)_n$@Ni_2(dobdc). At pH = 1.8, the acidified MOF yields a proton conductivity of 2.2×10^{-2} S cm^{-1} at 80 ^{o}C and 95% relative humidity (RH), which is commensurate with the highest values reported for MOFs. Proton conduction occurs via the Grotthuss mechanism among the proton-conducting MOFs. Protonated water clusters within the pores of $H^+(H_2O)_n$@Ni_2(dobdc) play an important role in the conduction process.

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Amine-functionalized MOF with exceptionally high CO_2 capture

이우람 홍창섭*

고려대학교 화학과

A framework en-Mg_2(dobpdc) (1-en; en = ethylenediamine) functionalized with the primary diamine en was prepared via postmodification. 1-en is demonstrated to great uptake of CO_2 13.7 wt % at 150 mbar and ambient temperature. These conditions are notably apt for post-conbustion capture. The CO_2 capacity of 1-en at 0.39 mbar is 11.1 wt %, which records the highest amount among MOFs for CO_2 capture. The isosteric heats of adsorption of 1-en in CO_2 capture corresponds to -51 kJ/mol, which is supported by DFT calculations (-52.8 kJ/mol). These results indicate that the adsorption of CO_2 onto the free amines of en leads to the formation of a carbamic acid. The CO_2 adsorption rate in 1-en is highest when compared with the well known MOFs for CO_2 capture. Desorption-regeneration cyclings of CO_2 at the simulated air(0.39 mbar CO_2) and flue gas(150 mbar CO_2) are established with almost retaining CO_2 capacities, which could provide great potential for practical application in CO_2 capture. The recyclability in CO_2 uptake for 1-en is maintained even after exposure to 99.9% relative humidity. The structures and sorption properties of 1-en will be presented in detail.

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M(diphosphine)(1,2-dithiolene) Complexes With M = Ni(II) and Pt(II): Comparison of Electrochemical Behaviors

이윤경 박태정 노동윤*

서울여자대학교 화학과

The (P-P)Ni(1,2-dithiolene) complexes where P-P is 1,2-bis(diphenylphosphino)ethane (dppe) and 1,1'-bis(diphenylphosphino)ferrocene (dppf), were synthesized using (P-P)$NiCl_2$ and the 1,2-dithiolene ligands such as 1,3-dithiole-2-thione-4,5-dithiolate (dmit), 1,2-benzenedithiol (bdt) and maleonitriledithiolate (mnt). X-ray structural analysis for (dppe)Ni(dmit) shows that the P_2NiS_2 core is a highly distorted square planar geometry, compared with the Pt(II) analogue, with S(1)S(2)P(2)P(1) torsion angle of 27.2^o. (Fig. 1(left)) In the cyclic voltammograms for (dppf)Ni(dithiolene) complexes, oxidation potentials for Ni(II) and ferrocene are very closed each other at an anodic potential region while the reduction of Ni(II) appears at a cathodic region. Two oxidation peaks of the phosphine moieties are observed in dppf complexes, but one oxidation peak (Fig. 1(right)) is observed for dppe complex. These electrochemical behaviors for Ni(II) complexes are totally comparable to the corresponding Pt(II) analogue, which will be presented in detail.

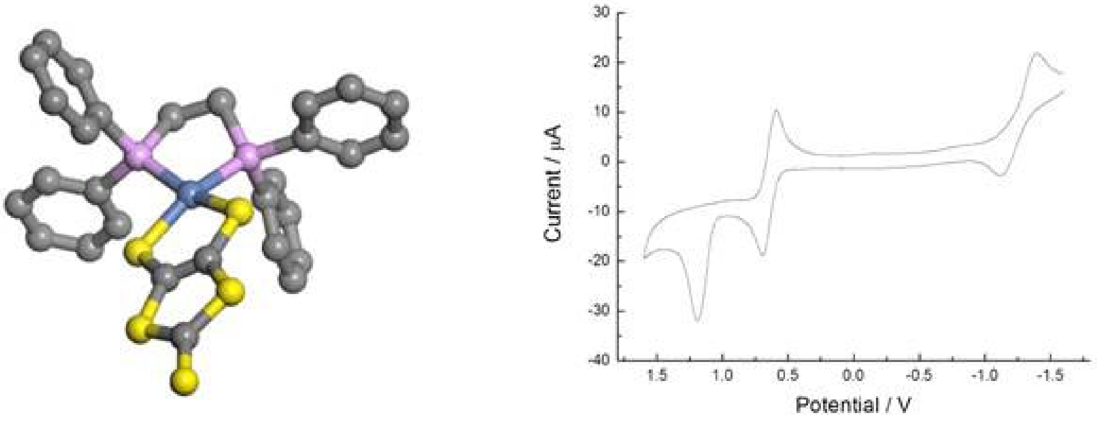

Fig.1. Molecular structure (left) and CV (right) of (dppe)Ni(dmit).

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Synthesis, structure and sorption properties of a two-fold interpenetrated 3D metal-organic framework

정소연 임광수 홍창섭[*]

고려대학교 화학과

Metal-organic frameworks (MOFs) are high porous materials and have application in gas sorption, storage and separation because of high surface area. We designed a new tripodal ligand, H_3L [= 4',4'',4'''-nitrilotris(3-methoxybiphenyl-4-carboxylic acid)] with methoxy pendant group. The reaction of H_3L, 4,4'-bipyridine, and Zn(II) allows for the formation of a 3D MOF with 2-fold interpenetration. Each zinc atom is coordinated with three L^{3-} molecules and one 4,4'-bipyridine molecule. We will present the detailed structure and sorption properties.

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CO_2 capture capabilities and structural variation in M_2(dobpdc)

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고려대학교 화학과

Metal-organic frameworks with Lewis acidic sites have been highlighted because of their gas capturing properties. We prepared a series of M_2(dobpdc) (M = Mg^{2+}, Mn^{2+}, Co^{2+}, Ni^{2+}, Zn^{2+}; $dobpdc^{2+}$ = 4,4′-dioxido-3,3′-biphenyldicarboxylate) to elucidate correlation between CO_2 binding affinity and structural parameters. The series feature 3D frameworks with hexagonal 1D channels running along the c axis. We will present the detailed study of structural and sorption properties for the extended MOFs.

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Control of microporosity and polarity on synthetic carbon adsorbents for increased CO_2 capture capacity

박우정 강민석 김동관 유원철*

한양대학교 응용화학과

The increase of CO_2 concentration in the atmosphere has been recognized as a major contributor to global warming, so people are greatly concerned about its environmental impact. CO_2 capture and storage is therefore necessary to prevent the release of large quantities of CO_2 into the atmosphere. Among the promising materials that could adsorb and store CO_2, carbon-based materials such as activated carbon, carbon nanotubes, nanofibres and templated carbon materials have been focused due to low cost, high chemical and thermal stability, and low sensitivity to moisture. For realizing high CO_2 adsorption property using carbon based materials, understand of structure-properties relations (i.e., microporosity, polarity and functionality) of carbon materials are essential. Herein, we investigate CO_2 adsorption capacity of synthetic carbon materials (e.g., 3D ordered macro/mesoporous (3DOM/m carbon), mesoporous carbon and etc.) in terms of structure-properties of synthetic carbon materials. Using various methods to control the microporosity and polarity (mainly the extent of oxygenates and nitrogen based moieties on the carbon), it is elucidated how CO_2 capture on synthetic carbon materials is varied. Gas sorption measurements, SEM, TEM, IR, elementary analysis and CO_2 adsorption experiments were carried out to prove the structure-properties relations of synthetic carbon materials for CO_2 capture.

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Study of diffusion-controlled photocatalytic activity by controlling pore size and particle size of TiO_2

이선화 박우정[1] 김동관[1] 강민석[1] 유원철[1,*]

한양대학교 응용화학 [1]한양대학교 응용화학과

TiO_2 is semiconductor that shows photocatalytic activity. Hence, it's been lots of investigations for increase of photocatalytic efficiency of TiO_2, mainly influenced by crystallinty, portion of specific crystalline plane expose, surface area, size of particle, etc. However, diffusion issue in liquid reactions in terms of sufficient interaction between reactant and surface of a photocatalyst has less been studied. So, we rationally design a phtocatalytic material that can be controlled with size of pore and particle size, key factors for determining the diffusivity of reactant under specific conditions. Here, we has synthesized three-dimentionally ordered mesopore (3DOm) TiO_2 for realizing the aforementioned issue. The *fcc* packed silica spheres (20-40 nm) were used as a template for preparing 3DOm TiO_2. The size of mesopore can be controlled by choosing the size of silica particle and the size of 3DOm TiO_2 can be tuned by controlling reaction condition. TiO_2 photocatalysts with mesopore sizes of 20-40 nm and particle sizes with 0.3-1 μm have been prepared to study the diffusion issue of Methylene Blue decomposition reaction under the specific conditions.

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Photocatalytic Activity of TiO_2 Pillared Layered Silicates Depending on Optical Transparency of 2D-Host

<u>PIAOHUIYAN</u> 양재훈 최진호*

이화여자대학교 화학.나노과학과

The porous photocatalyst was successfully synthesized by pillaring the titania nanoparticles in two dimensional layered silicates such as Kunipia-G (natural montmorillonite) and fluorine mica (synthetic swellable clay) through ion-exchange reaction and the consequent calcination. According to the X-ray diffraction analysis, the basal spacing of the TiO_2 pillared silicate layers were determined to be ~ 2.5 nm upon intercalation of TiO_2 nanoparticles, indicating that TiO_2 nanoparticles with the size of ~ 1.5 nm were successfully incorporated into the silicate layers to form the nanopore. From the nitrogen adsorption-desorption isotherms, the BET specific surface areas for the TiO_2 pillared Kunipia-G (TK) and the TiO_2 pillared mica (TM) calcined at 673 K were estimated to be 329 m^2/g and 266 m^2/g, respectively. The diffuse reflectance UV-vis spectra showed that the absorption edge of TiO_2 pillared layered silicates was blue-shifted compared to that of bulk anatase TiO_2 due to the quantum size effect of TiO_2 nano-particles stabilized in between the silicate layers. The photocatalytic activity of TM was significantly higher than that of TK for the photodecomposition of methylorange in the aqueous suspensions under UV irradiation, which would be systematically discussed with optical transparency of host layers.

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Synthesis, crystal structure and magnetic property of a Mn(III) azide complex

박민경 이우람 임광수 홍창섭*

고려대학교 화학과

Molecule-based magnetic materials have been studied for the potential applications in magnetic devices. We prepared Mn(III) complex $[Mn_2(L)_2(N_3)_3][Mn_2(L)_2(N_3)(H_2O)_2]$ (1) (H_2L = 6,6'-((1E,1'E)-(ethane-1,2-diylbis(azanylylidene))bis(phenylmethanylylidene))bis(3-(allyloxy)phenol), which contains two different types of Mn dimers bridged by single end-to-end azides. This complex has a two-dimensional layer structure involving hydrogen bonding. The detailed structural characterizations and magnetic properties will be presented.

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Synthesis of a new 2D metal-organic frameworks by extending the length of thiophene based ligand

<u>심수연</u>* 윤민영[1,*] 박경세[2,*] 이동헌[3,*]

가천대학교 글로벌캠퍼스 바이오나노학과 [1]가천대학교 글로벌캠퍼스 화학과 [2]군산대학교 화학과 [3]전북대학교 화학과

Metal-organic frameworks (MOFs) consist of metal ions and organic molecules as a node and as a linker, respectively. MOFs draw much attention because of its modularity and tenability. For instance pore size of MOFs can be modulated by changing the length of ligand. We have recently prepared a new 2,5-thiophenedicarboxylate (tdc) ligand based anionic MOF $[NH_2Me_2]_2[Cd(tdc)_2]$ (1). To increase the length of ligand, we have designed and synthesized 2,2’-bithiophene-5,5’-diacarboxylic acid (btdc), which has one more thiophene unit. Under the same reaction condition, we have successfully synthesized $[Cd_2(btd)_2(DMF)_2]\cdot DMF\cdot H_2O$ (2). Single crystal X-ray structure analysis showed the resulting MOF has a 2D Brick structure, which has an ABA packing structure. Unlike our expectation, the resulting framework structure of 2 was not an isostructure of 1. Details of our recent work will be presented.

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방향성 아민 유도체 검출을 위한 크라운 에테르와 칼릭스아렌이 도입된 CdS 및 Ag 나노입자 제조

백영은 안준호 정종화*

경상대학교 화학과

본 연구에서는 방향성 아민 유도체를 검출하기 위해서 싸이오펜이 도입된 크라운 에테르와 카복실기가 도입된 칼릭스 아렌을 합성하였다. 그리고 수용액에서 호스트 분자로써 크라운 에테르 유도체는 CdS 나노입자에 고정화 시켰으며, 칼릭스아렌 유도체는 Ag 나노입자 표면에 고정화 시켰다. 이렇게 합성된 CdS 와 Ag 나노입자를 이용하여 방향족 아민 유도체의 검출에 대한 연구를 수행하였다. 그 결과, 두 나노입자 수용액에 방향족 아민이 존재시에는 CdS 나노입자의 형광이 크게 감소하였다. 이는 방향족 아민 유도체의 벤젠부분이 칼릭스아렌 유도체와 결합하고, 아민 부분이 크라운 에테르 부분과 결합하기 때문이다. 따라서 본 연구에서는 크라운 에테르와 칼릭스아렌이 도입된 CdS 및 Ag 나노입자를 제조하여 방향성 아민족 물질을 선택적으로 검출하는 체계를 구축할 수 있었다.

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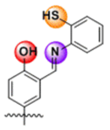
Benzothiazole-BODIPY conjugation mediated Cu+/Cu2+ and fluorescence probing: “turn-on” responses via solvent tuning to eliminate Hg2+ interference

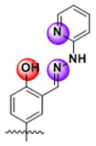
정정아 D.G.Churchill[*] 전태홍 MANJARESUDESHTULSHIRAM[1]

한국과학기술원(KAIST) 화학과 [1]기초과학연구원(IBS) 분자활성 촉매반응 연구단

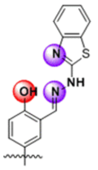
Herein, we will introduce novel conjugation that involves benzothioimidazole substitution to a salicylaldehyde-functionalized BODIPY system. Important and unexpected chemosensing “turn on” response patterns were discovered for copper ion which were found to be solvent-dependent. These percentage changes of aqueous solvent (CH3CN : H2O) can be tuned to allow for clear and major fluorescence increases for both Cu+ and Cu2+ which can almost completely eliminate the Hg2+ competitive signal.



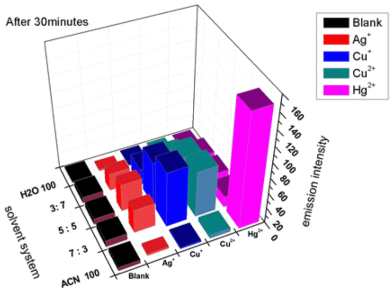
Copper-dependent cysteine / over homocysteine



Zinc-dependent PPi detection



MeCN-dependent Cu selectivity over Hg2+



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Anisotropic Liquid Phase Deposition of SiO2 on Hexagonally Close-packed Silica Beads

윤서영 이진석*

숙명여자대학교 화학과

Liquid phase deposition (LPD) is a useful method for the deposition of oxide films at low temperatures under aqueous conditions. LPD research has focused on the formation of oxide film, particularly its thickness, density, and composition.In this work, we synthesized the silica beads with the St?ber method and organized them into hexagonally close-packed monolayer using the Langmuir-Blodgett method. On this substrate, we conducted the LPD process with different saturation of hydrofluorosilicic acid and achieved different topography of silica beads. This was accomplished by competing deposition and etching reaction. And we proposed a mechanism for anisotropic liquid phase deposition on nanostructured surface. The advantage of these local reactions occurring on the nanostructured surface is the production of building blocks with distinctive shapes, which cannot be produced with conventional methods. Furthermore, the nanostructures could be useful in the bio-interface field as a substrate that influences biological systems.

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Development of Hole-Transporting Materials for Inorganic?Organic Hybrid Perovskite Solar Cells

최혜주 도광석 이혜정[1] 고재중*

고려대학교 소재화학과 [1]고려대학교 세종캠퍼스 소재화학과

Increasing energy demands and environmental issues such as fossil fuel shortage and global warming have leads to the need for clean renewable energy. The CH3NH3PbI3 perovskite is used as light harvesters for solar cells. The sensitized solar cells based on perovskite with the advantages of low-cost and high efficiency have the potential to be the ideal photoelectric conversion device. In mesoscopic solar cells using perovskites, spiro-OMeTAD and several conducting polymers have been used as HTMs. However, the HTMs have problems of high cost and/or low performance. Here we report the synthesis and characterization of new HTMs, and their application in perovskite-based solar cells.

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A fused amine core and propenylbenzene side arms: Efficient, Easily Obtainable, and Inexpensive Hole-Transporting Materials

<u>박소진</u> 도광석 최혜주 조현준[1] 이혜정[1] 고재중*

고려대학교 소재화학과 [1]고려대학교 세종캠퍼스 소재화학과

Organic material devices are attractive because they can take advantage of low molecular weights, potentially low cost, and capability for thin-film, large-area, flexible device fabrication. All the devices described above involve charge transport as an essential operation process, and hence, require proper charge-transporting materials. Therefore, the development of high-performance, charge-transporting materials is a key issue for the fabrication of high-performance devices.So we set up to Star-shaped charge-transporting materials with a fused amine core and propenylbenzene side arms. It was obtained in short step synthetic procedure.In this study, we try to determine the properties and characters of the compound through a various measurement.

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

도광석 박소진 조현준[1] 고재중*

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

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Direct Evidence of Forster Resonance Energy Transfer for the Enhanced Photocurrent Generation in Dye-Sensitized Solar Cell

최혜주 도광석 조현준[1] 고재중*

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Sensitization of wide band gap semiconductor surface by covalently grafting sensitizers such as polypyridyl ruthenium and organic dyes is central in applications to solar energy conversion in dye-sensitized solar cells (DSSCs). Essential for efficient conversion of solar energy by DSSCs is the development of panchromatic sensitizer which covers the whole solar radiation. Therefore, the development of optimal sensitizer, which combines the broad spectral coverage from 400 to 800 nm with a proper excited-state energy for favorable electron-transfer dynamics is a primary target. In the second approach, the simultaneous adsorption of the multiple dyes with complementary absorptions in the visible region was utilized to achieve the panchromatic sensitization of DSSCs. However, the drawback of such a technology is the limited number of sites on the TiO2 films for anchoring the dyes. To supplement this point, Durrant et al. and Choi et al. introduced the stepwise cosensitization of TiO2 films utilizing Al2O3 layers. A third approach is to use the concept of inter- or intramolecular energy transfer based on Forster Resonance Energy Transfer (FRET). The former developed by McGehee et al. proposes to use an unanchored energy relay dyes (ERD) dissolved in the electrolyte which acts as an energy donor molecule to the sensitized dyes (SD) anchored on the TiO2 films. However, as the FRET rate is a function of the distance between the ERD and the SD acceptor molecule, an efficiency enhancement could be modest because the separation distance between ERD/SD array is large enough. The latter is made of covalently linked donor dye, so-called “antenna unit” and the chemisorbed acceptor sensitizer, showing an enhanced photovoltaic performance in DSSCs due to the broad spectral coverage. As an extension of this concept, Odobel et al. described the facile assembly of panchromatic sensitizer formed through a coordinative interaction of chromophoric unit and a zinc porphyrin sensitizer. The incorporation of antenna unit to the porphyrin covers a wide window of the solar spectrum and shows a remarkable improvement to antenna-free systems.

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Perovskite solar cells using new hole transporting materials

도광석 박소진 고재중*

고려대학교 소재화학과

Thin-film photovoltaics play an important role in the quest for clean renewable energy. Recently, methylammonium lead iodide perovskites were identified as promising absorbers for solar cells. Hole-transport-material (HTM) usually used Spiro-OMeTAD and poly(triaryl amine) (PTAA). When these HTM use solid electrolyte, they obtained about 15% of power conversion efficiency. However, they have many problems and have to carry on a discussion of many issues for commercialization. They have no competitive price because of difficult purification, synthetic process, and batch-to-batch problem. Here, we design and syntheses of new hole transporting materials. By obtaining a high efficiency, we can open new research field.

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Molecular Layer Deposition of Organic-Inorganic Nanohybrid Thin Films using TMA and alkanediols

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한양대학교 화학과 [1]숙명여자대학교 화학과

We fabricated organic-inorganic nanohybrid thin films using trimethylaluminum and alkanediols by a sequential, self-limiting surface chemistry process known as molecular layer deposition (MLD). Using ellipsometry, we confirmed linear growth of the films versus number of MLD cycles at all same temperature. Atomic force microscopy was also used to check the roughness of the films that showed the roughness increased with increasing of the number of alkyl chains. Contrary, the film density decreases with increasing of the number of alkyl chains.

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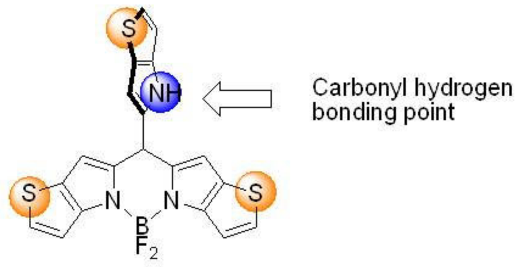
BODIPY species containing thieno-pyrrole groups: consideration of a new type of β-sheet formation fluorescent probe with external 5-membered rings and a NH group

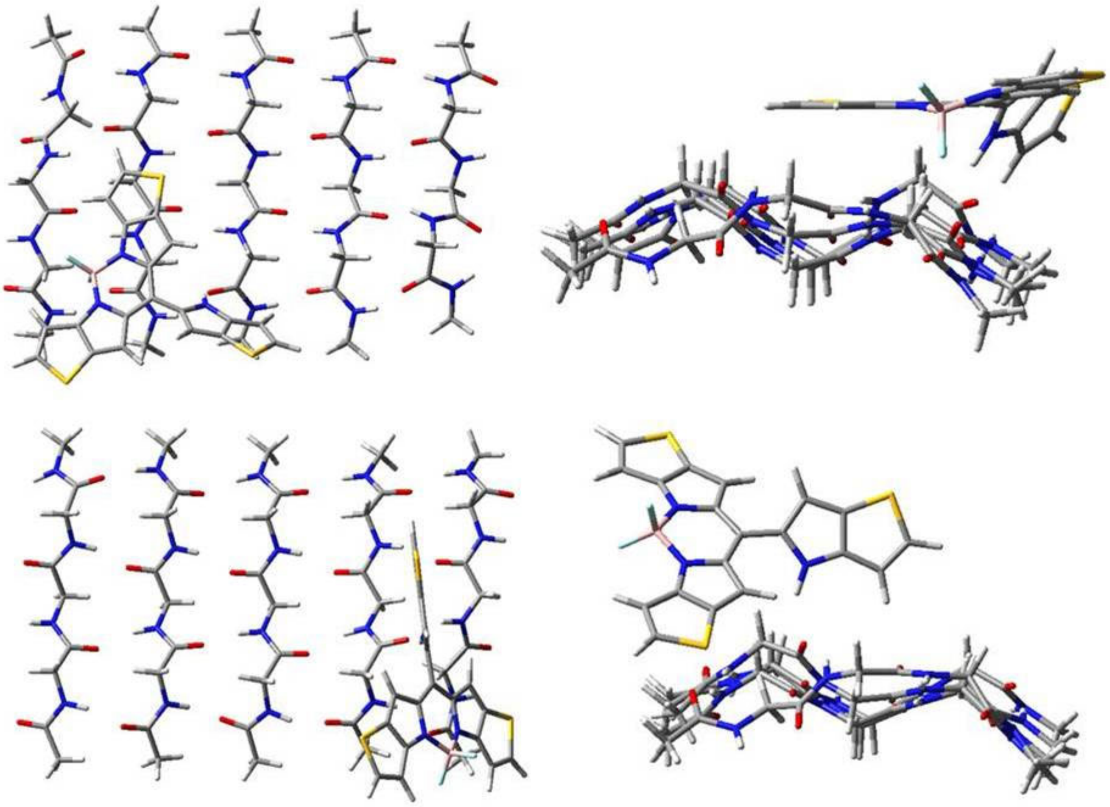
<u>전태홍</u> MANJARESUDESHTULSHIRAM[1] 이윤섭 D.G.Churchill[*]

한국과학기술원(KAIST) 화학과 [1]기초과학연구원(IBS) 분자활성 촉매반응 연구단

A series of related BODIPY species involving the novel thieno-[3,2-b]-pyrrole system have been prepared studied structurally, photophysically, and computationally. The idea is put forth that a (i) planar fluorophoric compound composed of all non-core rings to be 5-membered and an (ii) [NH] heteroatomic group poised on the aryl rotor might allow for decent responsiveness upon β-sheet binding groove (below). Thus, we can follow this design as a reasonable prototype in small molecular β-sheet binding. In the crystal structure of our main fluorogenic compound (below), the meso-position dihedral angle is slightly small. DFT theory was used to determine the potential energy surface of the ring rotation and model peptide carbonyl binding.



Carbonyl hydrogen bonding point



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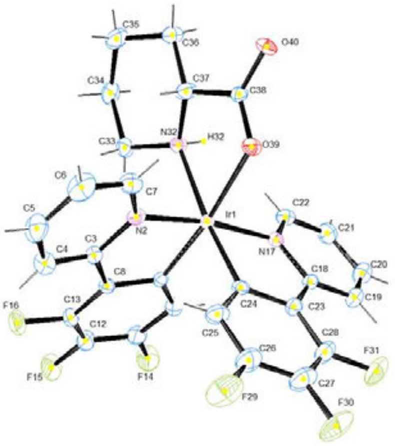
Phosphorescent Iridium(III) Complexes Based on 2-(2,3,4-Trifluorophenyl)pyridine for Organic Light?Emitting Diodes (OLEDs)

김민지 송영광 강성권[1] 김영인[2,*]

부산대학교 화학소재과 [1]충남대학교 화학과 [2]부산대학교 화학교육과

Cyclometalated iridium(III) complexes have received great attention because of their ability to achieve the theoretical upper limit of external quantum efficiency (η_{ext}) for red, green and blue phosphorescent organic light-emitting devices (phOLEDs). The cyclometalating ligands for efficient green phorescent iridium(III) complexes were synthesized and characterized ; $(tfppy)_2Ir(pipec)$ (1), $(tfpmpy)_2Ir(pipec)$ (2), $(tfppy)_2Ir(prl)$ (3) and $(tfpmpy)_2Ir(prl)$ (4), where tfppy = 2-(2,3,4-trifluoromethyl)pyridine, tfpmpy = 4-methyl-2-(2,3,4-trifluoromethyl)pyridine, pipec = pipecolinic acid and prl = L-proline. The structures were determined using single crystal X-ray method and revealed that complexes 1 and 2 adopted distorted octahedral geometries around iridium metal ion with cis-C, C and trans-N, N positions. The phosphorescence properties of complexes 1~4 showed green emission at 488~495 nm in PL spectra and exhibited quantum yield of 28~42 % in dichloromethane solution. The EL device of compound 2 show the best performance with external quantum efficiency of 7.76%, luminance of 1822 cd m^{-2}, the maximum current efficiency of 21.75 cd A^{-1} and commission international de’Eclairage coordinates of (0.23, 0.53).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C36
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C34
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O39
C6
C7
C5
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C21
C3
N17
C4
C20
C8
C18
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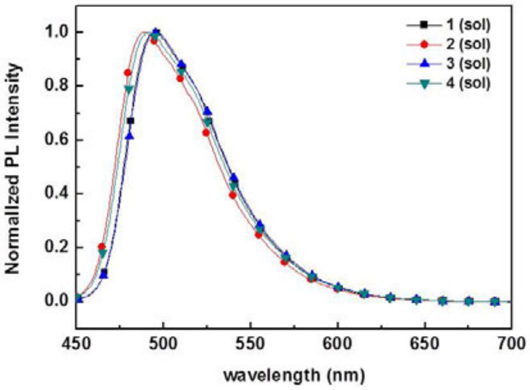
1 (sol)
2 (sol)
3 (sol)
4 (sol)
Normalized PL Intensity
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0.6
0.4
0.2
0.0
450
500
550
600
650
700
wavelength (nm)

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Synthesis of Porous Coordination Network Using a Multi-Redox-Centered Ligand

하주연 **Masaki Kawano***

포항공과대학교 첨단재료과학부

In the field of porous coordination networks, how to design ligands is crucial for introducing physical properties like redox-activity; it can induce electrical conductivity, magnetism, and so on. We have newly synthesized redox-active as well as multi-interactive ligand 5,5',8,8'-tetra(4-pyridyl)-2,2'-(1,4-phenylene)bis-1H-perimidine which contains two redox active sites. It can show several electronic states based on two diazaphenalenyl moieties which are connected by phenylene unit. Therefore, its coordination compounds can show mixed valence states which cause unique physical properties. In this presentation, we will report a new network structure composed of the ligand and metal ions and its basic electronic properties.

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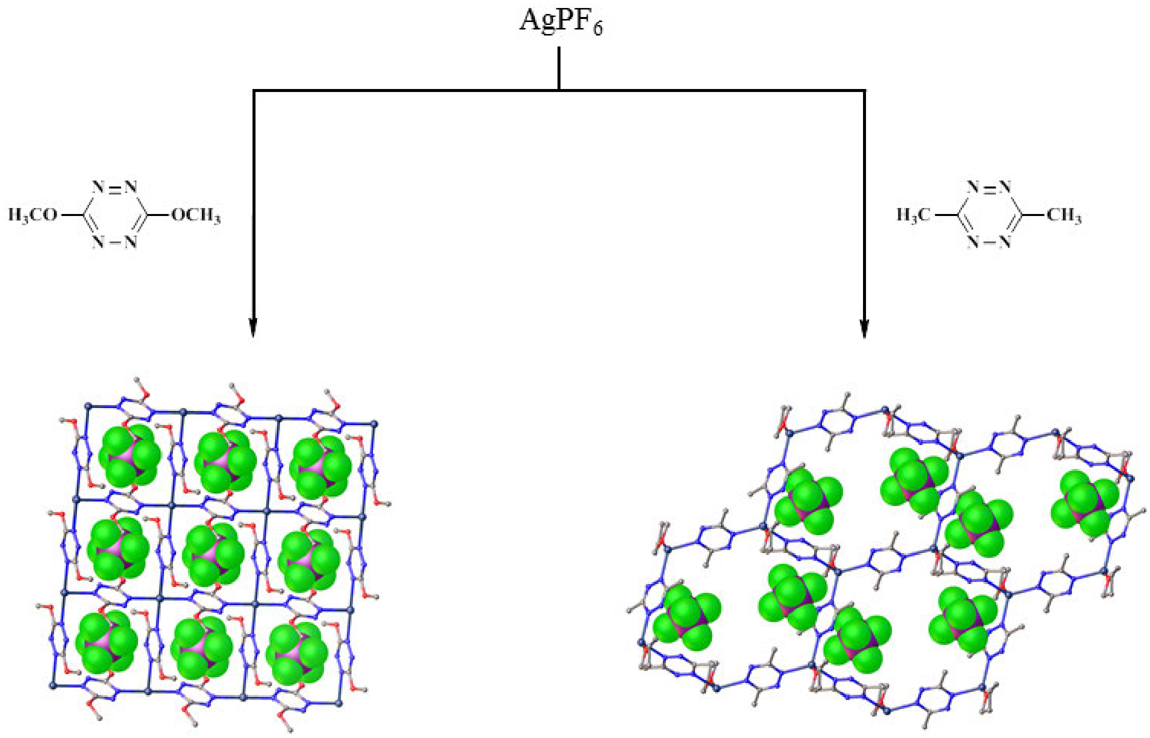
Synthesis and Structural Analysis of 3,6-Disubstituted s-Tetrazine Silver Complexes

강필재 오한솔 강혜지 최문근*

연세대학교 화학과

The unique characters of s-tetrazines, the nitrogen-rich six-membered aromatic heterocycles originate in their extreme electron deficiency. The electron deficiency of the π-system enable to sustain efficient attraction for polarized atoms or anions. Another important property of tetrazines is that since it has the multiple metal binding sites, it makes transition metal complexes easily with multinuclear coordination complexes.Coordination polymers and metallamacrocycles containing s-tetrazine derivatives and hexafluorophosphate with novel topology are synthesized and their X-ray crystal structural features will be presented. Especially taking into account the influence of anion-π interaction with various of 3,6-disubstituted derivatives to generate new supramolecular architectures.


$AgPF_6$
H₃CO, N=N, N–N, OCH₃
H₃C, N=N, N–N, CH₃

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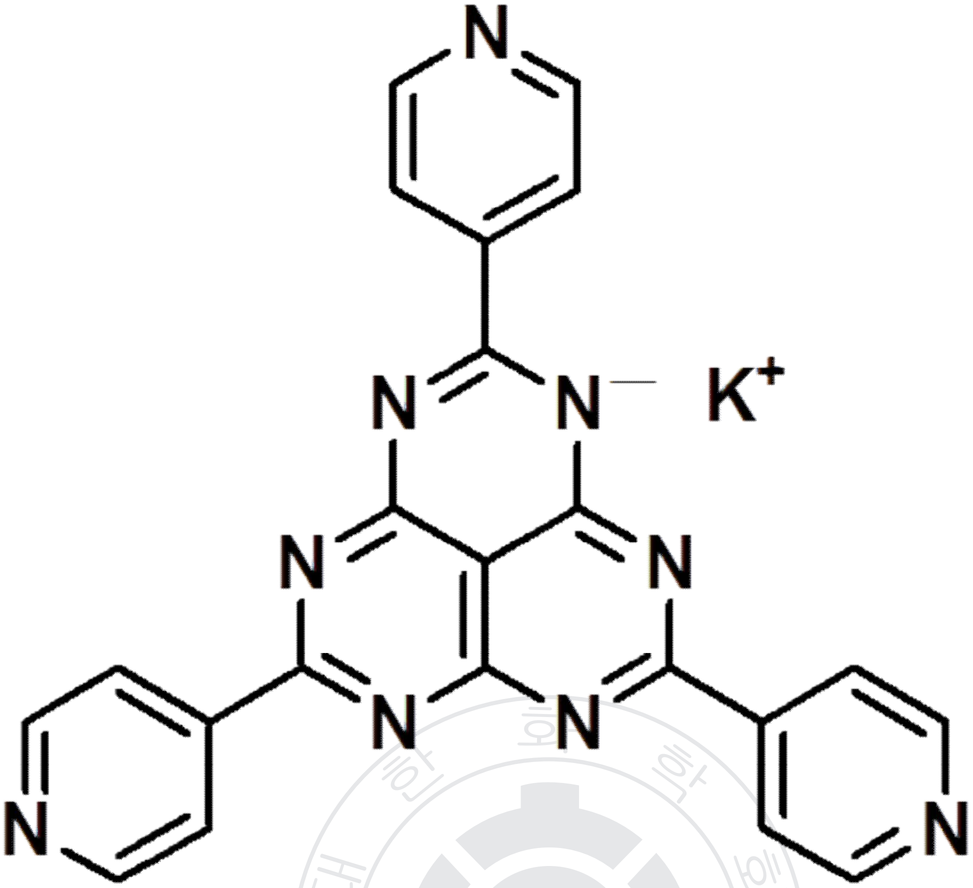
Ionic Conductor based on Multi-interactive Organic Molecule

이길령 **Masaki Kawano***

포항공과대학교 첨단재료과학부

Preparation of efficient ion conducting system is one of the most attractive fields in the material chemistry. Although still there are many problems to be solved, recent efforts from various fields have been overcoming them. However, the detailed structural information of conductive phase especially in polymer based conductor is essential to provide better understanding of conduction event and the strategy for the design of efficient conductive system. Recently, we have successfully revealed the structure of conduction path in the self-assembled soft structure of newly synthesized multi-interactive molecule, tris(4-pyridyl)hexaazaphenalene (TPHAP) by ab initio XRPD method. The potassium salt of TPHAP showed high ion conductivity up to 3.4 x 10^3 S/cm by fully hydration. This high conductivity was realized by the large water channel formation which is stabilized by weak intermolecular interaction between TPHAP and water molecules. Our materials can be good models for understanding the conduction mechanism of soft materials like polymer. Here, we extend our study to different counter cation system and discuss the effects of them for the ion conductivity and the structure.



TPHAP potassium salt

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In Situ Monitoring and Analysis on Interactions between Nanoarticles on Supported Lipid Bilayer

김선기 남좌민*

서울대학교 화학부

Observing individual nanoparticle reactions provides direct information and insight for many complex reaction processes, but this is challenging with conventional high-resolution imaging techniques on conventional platforms. Here, we developed a plasmonic nanoparticle-modified supported lipid bilayer (PNP-SLB) platform and single-particle imaging method that allow for massively parallel and quantitative in situ analysis of the interactions between nanoparticles. We also show the use and applications of this method for the study on inter-particle reaction kinetics and micropattern-based DNA detection assays with multiplexing capability.

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Physical properties of redox-active porous coordination network

김재준 **Masaki Kawano***

포항공과대학교 첨단재료과학부

Proper ligand design is crucial for realization of porous coordination network which can show unique physical properties such as conductivity, magnetism, optical characteristics. Especially, the ligands having multi-interactivity and/or redox activity are attractive in terms of trapping metastable state during self-organization and introduction of redox activity to coordination network. Recently we designed and synthesized redox active ligand, 2,5,8-tris(4-pyridyl)-1H-perimidine (TPDAP). We confirmed that TPDAP shows irreversible 2-step oxidation processes by cyclic voltammetry measurement. Considering this result and multi-interactivity of TPDAP, it is expected that TPDAP can give various kinds of redox-active porous networks. Here, we show our recent work of porous coordination network composed of TPDAP and cadmium nitrate.

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Altering and Controlling Amyloid-β Aggregation with Plasmonic Nanoparticles on Brain-Mimicking Lipid Bilayer

김유나 이효진[1] 남좌민*

서울대학교 화학부 [1]Department of Chemistry, Northwestern University, USA

It is widely accepted that large amyloid β (Aβ) aggregates are one of the hallmarks of Alzheimer's disease (AD), and study on Aβ aggregation and its impact on AD would be beneficial to diagnosis and cure of AD. Here, we studied the formation of various Aβ aggregate structures with gold nanoparticles (AuNPs) with plasmonic optical properties and brain total lipid extract-based supported lipid bilayer (brain SLB). AuNPs were added for monitoring the structural details of Aβ aggregates by analyzing structures with the dark-field imaging of plasmonic AuNPs that allows for long-term in situ imaging of Aβ aggregates with great structural details without further labeling. When Aβ were coincubated with AuNPs on brain SLB, Aβ peptides were aggregated into plaque-like structures with dense cores, which means that AuNPs and brain SLB synergistically affect to the formation of large Aβ aggregate structures such as Aβ plaques.

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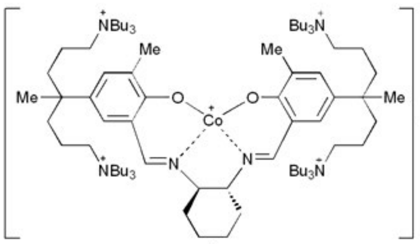
Highly active salen-cobalt(III) complex tethering 4 quaternary ammonium salts and it's ligand study

전종엽 이분열*

아주대학교 분자과학기술학과

Recently, a high active catalyst for CO2/epoxide copolymerization was developed in our group. This Co(III) complex (1) contains salcy-type ligand tethering four quaternary ammonium salts1,2 The related cobalt(III) complexes 2?5 were prepared through variations of the ligand framework of 1 by replacing the trans-1,2-diaminocyclohexane unit with 2,2-dimethyl-1,3-propanediamine, trans-1,2-diaminocyclopentane, or 1,1′-binaphthyl-2,2′-diamine or by replacing the aldimine bond with ketimine. These ligand frameworks are thought to favor the formation of the cis-β configuration in complexation, and the formation of the cis-β configuration in 2?5 was confirmed through NMR studies or X-ray crystallographic studies of model complexes not bearing the quaternary ammonium salts. Complexes 2, 4, and 5, which adopt the cis-β configuration even in DMSO did not show any activity for CO2/PO copolymerization. Complex 3, which was constructed with trans-1,2-diaminocyclopentane and fluctuated in DMSO between the coordination and de-coordination of the acetate ligand as observed for 1, showed fairly high activity (TOF, 12 400 h?1). This fluctuating behavior may play a role in polymerization. However, complex 3 did not compete with 1 in terms of activity, selectivity, and the catalyst cost.



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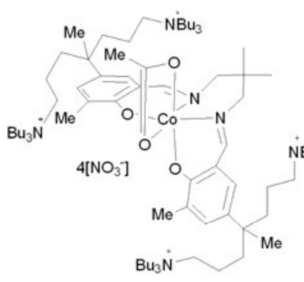

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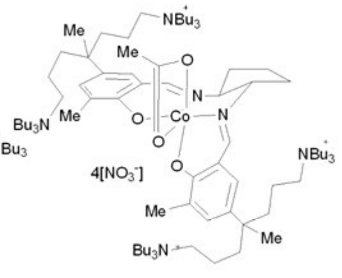

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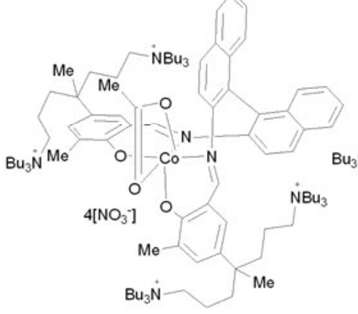

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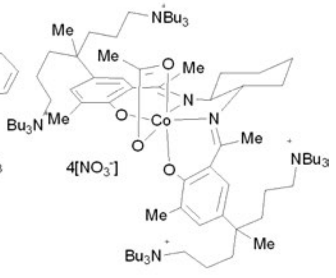

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Structural and Photoluminescence Properties of Copper(I) Coordination Polymers Based on Dithioether Ligands with Pyromellitic Diimide

강기행 이상진 조성화 전영은 김태호 김진은*

경상대학교 화학과

Four copper(I) coordination polymers (CPs) have been synthesized by the reaction of CuI and two dithioether ligands N,N'-bis[2-(*t*-butylthio)ethyl]pyromellitic diimide, (L^1) and N,N'-bis[2-(benzylthio)ethyl]pyromellitic diimide (L^2). Structural and photophysical studies of CPs 1-4 in solid state are reported. Coordination polymers 1-4 are composed of cubane Cu_4I_4 cluster nodes, emitting red-orange light under UV-irration. The results of our investigation including syntheses, structural characterization, thermal and photoluminescent properties of four new Cu(I) coordination polymers are presented.

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Controlled Reversible Crystal Transformation of Cu(I) Supramolecular Isomers and Pseudopolymorphs

전영은 조성화 이상진 강기행 김태호 김진은*

경상대학교 화학과

Four copper(I) coordination polymers (CPs), $\{[\mathrm{CuIL}]\cdot\mathrm{CH_3CN}]\}_n$ (1), $\{[\mathrm{CuIL}]\cdot\mathrm{CHCl_3}\}]\}_n$ (2), $\{[\mathrm{CuIL}]\cdot\mathrm{CH_2Cl_2}\}]\}_n$ (3), and $[\mathrm{CuIL}]]\}_n$ (4), have been prepared by self-assembly reaction between CuI and (2-pyrazinylcarbonyl)thiomorpholine (L). CPs 1-4 are interconnected by rhomboid Cu-$\mathrm{I_2}$-Cu units. CPs 1 and 4 have 1-D loop-chain structures and 2 and 3 adopt 2-D network structures. CPs 1-4 are supramolecular isomerers by solvent molecules. CPs 2' and 3' are prepared by removal of solvate molecules from CPs 2 and 3, which are polymorphs with CP 4. Reversible crystal-to-crystal transformations were observed under appropriate conditions such as solvent or heat.

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Versatile Cu_xI_x Cores in Cu(I) Superamolecular Isomers Based on N/S Hetero Donor Ligand; Reversible Crystal-to-Crystal Transformation

조성화 이상진 전영은 강기행 김태호 김진은*

경상대학교 화학과

Controlled self-assembly of CuI and an asymmetric ligand 2-(*t*-butylthio)-*N*-(pyridin-3-yl)acetamide (**L**) with mixed N/S donor set, afforded five copper(I) superamolecular isomers $[Cu_2I_2\mathbf{L}_2]_n$ (**1**), $[Cu_4I_4\mathbf{L}_2]_n$ (**2** and **3**), $[Cu_4I_4\mathbf{L}_2(CH_3CN)_2]_n$ (**4**), and $\{[Cu_4I_4\mathbf{L}_2]^{\cdot}CH_3OH\}_n$ (**5**). X-ray analyses of **1**-**5** show diverse Cu_xI_x cluster cores, rhomboid Cu_2I_2 (**1**), cubane-like Cu_4I_4 (**2**, **3** and **5**), and stair-step Cu_4I_4 (**4**). Transformation between **3** and **4** is an example showing reversible crystal-to-crystal transformation between Cu_xI_x cluster cores, controlled by heat and MeCN solvent. Also, **5** was transformed to **4** by addition of CH_3CN. Complexes **1**, **2**, **3**, **4**, and **5** emit blue, red, yellow, bright blue, and green yellow color light under UV-irradiation, respectively.

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Synthesis and Characterization of Copper(Ⅰ) Coordination Polymers Based on Pyrazine Ligands with Thioether Substituents

이상진 조성화 전영은 강기행 김태호 김진은*

경상대학교 화학과

The N/S Mixed donor ligands (L^1 and L^2) were synthesized by the reaction of 2-pyrazinecarbonyl chloride and $RSCH_2CH_2CH_2NH_2$ (R=benzyl, cyclohexyl). Cu(I) coordination polymers $[CuIL^1]_n$ (1), $[Cu_3I_3L^1]_n$ (2), $[CuIL^2]_n$ (3), and$[Cu_4I_4L^{2}2]_n$ (4) were prepared by the reaction of CuI and ligands. CP 1 shows a 2D network structure, based on rhomboid Cu_2I_2 node. CP 2 has mixed core units rhomboid Cu_2I_2 and cubane Cu_4I_4. CP 3 shows an interpenetrate 3D network structure. CP 4 has cubane Cu_4I_4 units. We report structures, thermal behaviors and photophysical properties of the coordination polymers based on N/S mixed donor ligands.

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Photochemical Hydrogen Production Using Rh Complexes and Pt Nanoparticles: Effect of Nicotinamide

김진홍* 김수진[1]

이화여자대학교 화학·나노과학과 [1]이화여자대학교 화학나노과학과

Photochemical hydrogen production is carried out using platinum nanoparticles (PtNPs) and visible light energy with chemically generating rhodium-hydride species from molecular Rh complexes and sodium formate. Rh-hydrides not only reduce NAD+ to generate NADH, but also react with protons by photoactivation in the presence of PtNPs to produce H2. The chemically generated NADH is sequentially photoactivated by PtNPs and eosin Y to produce hydrogen. These two hydrogen production pathways show different rate-limiting steps based in kinetic studies using Rh catalysts containing electron-donating and electron-withdrawing groups.

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Detection of Cyanide, Magnesium, Zinc Ions by Fluorescent Chemosensor Containing a Dipyridylmethylamine Backbone

김진홍[*] 김 철[1,*] 김수진[2]

이화여자대학교 화학·나노과학과 [1]서울과학기술대학교 정밀화학과 친환경소재제품센터 [2]이화여자대학교 화학나노과학과

An assay to quantify the presence of cyanide, magnesium, and zinc ions with a chemosensor of dipyridylmethylamine coupled with coumarin was developed using a turn-on fluorescence enhancement approach. Upon treatment with magnesium ions, the fluorescence of the receptor at 365 nm was shifted to 408 nm and enhanced due to the formation of a complex between the receptor and magnesium ions at room temperature. As the concentration of Mg2+ was increased, the fluorescence gradually increased. Other metal ions, such as Na+, K+, Ag+, Ca2+, Mg2+, Zn2+, Mn2+, Co2+, Ni2+, Cu2+, Cd2+, Pb2+, Hg2+, Cr3+, Fe3+, Al3+ had no significant effect on the fluorescence.

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Cu^{II} complex synthesis, structure and characterization with Tetrathiafulvalene bis (4 (5) Carboxy-1, 3-dithiolidine)

KhanMohammadSherjeelJaved 조장훈 이주은 이홍인*

경북대학교 화학과

Tetrathiafulvalene (TTF) and its derivatives are renowned organic π donors which have been largely studied for distinct applications, in particular, in the area of conducting organic materials including intermolecular charge-transfer interactions with several π -accepting molecules (A). An array of mono- or polydentate coordinating functional groups has been adhered to the TTF moiety, and the interrelated metal complexes have been divulged. Tetrathiafulvalene (TTF) has proven to be an excellent electron donor in the preparation of highly conductive charge transfer compounds. The structural and electronic properties of TTF are considered to be important determinants of electrical-transport properties in crystals of conductive materials. Transition metal complexes are very helpful in the synthesis of charge transfer compounds because of change in their oxidation states by the adaptation of the chemical environments around the metal ions. In this study, we have done the synthesis of the transition metal coordination polymer containing a tetrathiafulvalene (TTF) moiety substituted with a dicarboxylic group of the formula [CuL] BCDT-TTF (L = 3,10-bis(2-hydroxyethyl)-1,3,5,8,10,12-hezaazacyclotetradecane) (BCDT = Bis(4,5-carboxy-1,3-dithiolidene). It has been characterized by various analytical methods.

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Reactivity of Nickel Monocarbonyl Species Supported by Diphosphinoamide Ligand with Alkyl Iodides

오서희 이윤호[1,*]

한국과학기술원(KAIST) 화학과 [1]KAIST 화학과

Carbon monoxide is one of the attractive C1 source because of its versatile usages in industrial processes such as hydroformylation and Monsanto process. Due to their excellent chemical and physical properties, most of current industrial CO transformation is generally catalyzed by noble metal catalysts. However, replacing such high valued catalysts by cheaper metallic elements is particularly attractive because of the economic advantages. According to recent reports, certain biological systems employ earth-abundant 1st row transition metals to utilize CO as their carbon source. In particular anaerobic bacteria, such as *Moorella thermoacetica*, Acetyl-CoA synthase (ACS) catalyzes the biosynthesis of acetyl-CoA from coenzyme A, a methyl group, and CO. The major chemical transformation including C-C bond formation takes place at a low-valent nickel center in the active site of ACS. Details of the mechanism, the order of substrate binding and the oxidation state of nickel are still in debates. For better understanding of the chemistry involved in ACS and ultimately developing the synthetic catalyst using organonickel complexes, the C-C bond formation chemistry of a low-valent nickel carbonyl species has been investigated. Recently, a nickel(II) monocarbonyl species supported by an anionic pincer-type PNP ligand ($PNP^- = N[2\text{-}P^iPr_2\text{-}4\text{-}Me\text{-}C_6H_3]_2$) was reported by our group. Here, we report the synthesis and characterization of corresponding mono-valent and zero-valent nickel monocarbonyl species. Due to the different number of d-electrons, a series of nickel monocarbonyl species revealed interesting differences in terms of their local geometry about nickel ion, bond strength and ultimately reactivity. In order to establish the organonickel C-C bond formation chemistry, particular reactivity toward iodoalkanes was carefully explored. From the electrophilic methylation, the Ni(I)CO species was transformed to a nickel acyl complex, $(PNP)NiCOCH_3$ via a C-C coupling, while Ni(0)CO species was converted to only $(PNP)NiCH_3$ via a ligand substitution. The detailed mechanistic studies are currently under investigations.

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New 2D Fluorescent Metal-Organic Framework Comprising Lanthanide and Conjugated Ligand

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가천대학교 글로벌캠퍼스 바이오나노학과 [1]가천대학교 글로벌캠퍼스 화학과 [2]군산대학교 화학과 [3]전북대학교 화학과

Metal-organic frameworks (MOFs) consist of metal ions and organic molecules as a node and as a linker, respectively. Usually MOFs are constructed by transition metal ion because it is easy to predict coordination geometry. However, for an application of the other property, such as fluorescence, lanthanides can be used. Herein we report new lanthanide based metal-organic framework, $[Eu_2(btd)_2(NO_3)_2(DMF)_2]\cdot 2DMF$ (2), comprising Europium and a new 2,2’-bithiophene-5,5’-dicarboxylate (btdc) ligand. Single crystal X-ray structure analysis showed the MOF has a 2D square grid structure with a ABC packing. UV-Vis absorption and fluorescence property of the framework was also studied. Details of our recent work will be presented.

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Synthesis and Crystal Structures of Copper(II) Complexes with 2-Acetylpyridine/2-Benzoylpyridine based Schiff Base Ligands

구본권

대구가톨릭대학교 생명화학과

Some new Cu(II) complexes of the type, $[Cu_2(L^{1\sim4})_2(HBA)]^+$(1~4) (L^1(1) = 2-acetylpyridine S-methyldithiocarbamate (acpy-mdtc$^-$), L^2(2) = 2-acetylpyridine 4-phenyl-3-thiosemicarbazate (acpy-phTsc$^-$), L^3(3) = 2-acetylpyridine benzhydrazide (acpy-bh$^-$), and L^4 (4) = 2-benzoylpyridine benzhydrazide(bpb$^-$) and HBA = benzilic acid) have been synthesized and characterized by elemental analysis, infrared spectroscopy, thermogravimetric analysis, and single crystal X-ray diffraction. The X-ray analysis reveals that the structures of 1 and 2 are dinuclear copper(II) complexes bridged by two thiolate sulfur atoms of Schiff base ligand and bidentate bridging HBA$^-$ anion. For 1, each of the two copper atoms has different coordination environments. Cu1 adopts a five-coordinate square-pyramidal with a N2OS2 donor, while Cu2 exhibits a distorted octahedral geometry in a N2O2S2 manner. For 2, two Cu(II) ions all have a fivecoordinate square-pyramidal with a N2OS2 donor. In each complex, the Schiff base ligand is coordinated to copper ions as a tridentate thiol mode.

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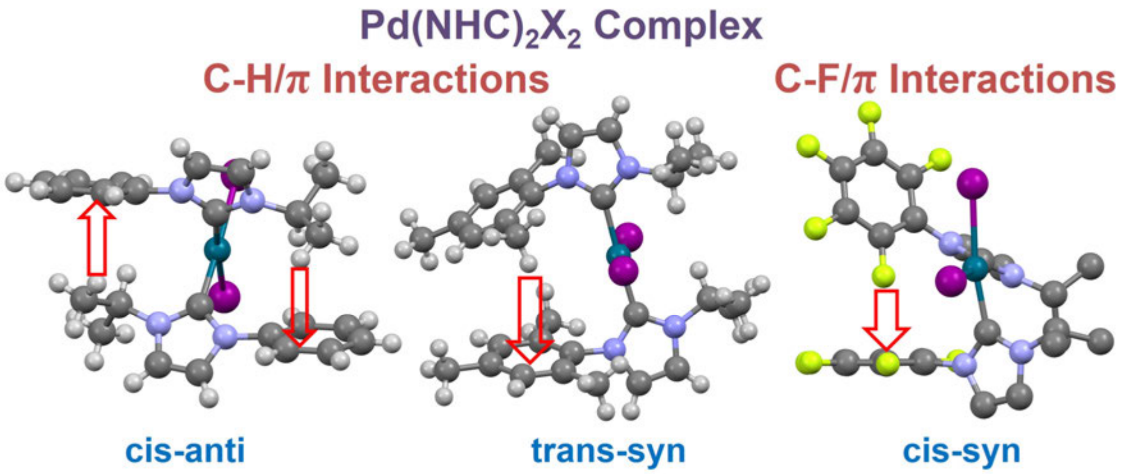
CH-pi and CF-pi Interactions Lead to Structural Changes of N-Heterocyclic Carbene Palladium Complexes

POOI MING SHURN BENJAMIN

서울대학교 화학

The role of CH-pi and CF-pi interactions in determining the structure of N-heterocyclic carbene (NHC) palladium complexes were studied using ^{1}H NMR spectroscopy, X-ray crystallography, and DFT calculations. The CH-pi interactions led to the formation of the cis-anti isomers in 1-aryl-3-isopropylimidazol-2-ylidene-based $[(NHC)_2PdX_2]$ complexes, while CF-pi interactions led to the exclusive formation of the cis-syn isomer of diiodobis(3-isopropyl-1-pentafluorophenylimidazol-2-ylidene) palladium(II).



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synthesis of Zinc complex with alkyl ligand

이병기 이익모*

인하대학교 화학과

aryl diketiminato Zinc complex is prepared and investigated for the copolymerizition of CO2/epoxide.in contrast zinc complex with alkyl ligand is not been studied well.for this reason, we were synthesised Zn complex with new alkyl diketiminato ligand.and using this complex,we will apply to copolymerization of CO2/epoxide.

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A highly selective fluorescent “turn-on” sensor for Fe^{3+} based on anthracene

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A novel fluorescent sensor 1 bearing one anthracene and two imidazole groups was easily synthesized and investigated for fluorescent sensing behavior by various metal ions. Anthracene-based fluorescent sensor 1 displayed highly selective and sensitive fluorescent “turn-on” toward Fe^{3+} in acetonitrile solution. Other ions including Ag^{+}, K^{+}, Li^{+}, Na^{+}, Ca^{2+}, Cd^{2+}, Co^{2+},Cu^{2+}, Ni^{2+}, Hg^{2+}, Zn^{2+} induced no or much smaller spectral changes. The 1:2 stoichiometry of sensor complex $1+Fe^{3+}$ was confirmed by Job’s plot based on fluorescence emission titration. Furthermore, the binding sites of sensor complex $1+Fe^{3+}$ was properly identified from ^{1}H NMR study.

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Theoretical study of additional cyclizations in a fluorinated polycyclic alkene via sigma-bond migration by DFT method

장효원

순천대학교 화학과

Alternatively fluorinated [16]annulenes may form weakly-binded stacked-layers aided by dipolar interactions induced by the oppositely polarized fluorine and hydrogen atoms, which, in turn, may be covalently bonded by forming intermolecular carbon-carbon sigma bonds connecting adjacent annulene rings. In this work, we pursue a part of such reaction pathways, along which the intermediates and transition structures involve biradical and diradical electronic characters, and also 1,2-sigma-bond migrations frequently. The reaction accompanies with about 200kJ/mol exothermicity, and with the highest barrier of about 280kJ/mol.

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Fabrication of Au@SiO_2 Core-Shell Nanowires from Linearly Assembled and Silica-Coated Gold Nanorods

정수경 장두전*

서울대학교 화학부

Gold nanorods have gained much attention for optical and optoelectronic devices, sensors, and biomedical technologies because of their rich SPR-derived properties. Recently, the techniques to create the assembly of gold nanorods have been studied to further enhance the applicability of gold nanorods since it shows unique properties such as the coupling of surface-plasmon resonances between the nanorods. In this study, the self-assembly of gold nanorods was successfully fabricated and further encapsulated with the silica shell and then the obtained silica-coated gold nanochains were welded into nanowires to produce Au@SiO_2 core-shell nanowires by irradiating infrared nanosecond pulses. Gold nanorods have been self-aligned by adding isopropanol without any assembling agents to form gold nanochains. The end-to-end assembled gold nanorods then have been directly encapsulated with uniform silica shells with tunable thickness to yield silica-coated gold nanochains. The nanosecond laser pulses of 1064 nm at fluence of 0.38 mJ/cm^2 have been applied to the obtained nanochains to fabricate Au@SiO_2 core-shell nanowires. This novel and straightforward synthetic approach to produce silica-coated gold nanowires has allowed gold nanowires to have strong near-infrared absorption, high stability, and easily functionalizable surface.

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Fabrication of anatase TiO2 nanotube arrays anodization of titanium in mixed viscous solvents

김형배 장두전*

서울대학교 화학부

Highly ordered, vertically aligned, one side-opened, and regularly porous anatase TiO2 nanotube arrays have been facilely grown by anodizing Ti foil in mixed viscous solvents of ethylene glycol and glycerol. By changing the volume ratio of two solvents, we have controlled the structural properties of TiO2 nanotube arrays such as tube diameters, wall thicknesses, and tube lengths. Our prepared TiO2 nanotube arrays have been found to have enhanced (004) planes, which are reactive in catalysis reactions. We have demonstrated that TiO2 nanotube arrays grown in 2:1 (v/v) ethylene glycol and glycerol have the lowest band-gap energy and the largest mean crystallite diameter. TiO2 nanotube arrays grown on Ti foil have been directly employed for photocatalytic materials and the working electrode of photovoltaic dye-sensitized solar cells. Among our prepared samples, TiO2 nanotube arrays grown in 2:1 (v/v) ethylene glycol and glycerol have shown the best photocatalytic activity for the degradation of methylene blue and the highest photovoltaic conversion efficiency of 4.08%.

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Facile-Growth Mechanism of Wurtzite ZnS Nanobelts

김연호 장두전*

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Despite recent achievements for the synthetic processes of wurtzite ZnS achieved from decomposition of $ZnS(en)_{0.5}$ (en = ethylenediamine) into ZnS via post thermal treatments, studying about the growth mechanism of $ZnS(en)_{0.5}$ into wurtzite ZnS is still challenging. Motivated by these needs, we have investigated their growth process through transmission electron microscopy, X-ray diffraction, thermal gravimetric analysis, X-ray photoelectron spectroscopy, and Fourier transform infrared spectroscopy with adjusting reaction conditions of the growth time, the growth temperature, and the applied solvent compositions. We have found out that en molecules have escaped from the lamellar structures of $ZnS(en)_{0.5}$ nanostructures through the interactions with water molecules at 180 ℃ for 6 h with proper amounts of water. The chemical composition, the morphology, and the optical properties of ZnS nanobelts have been controlled by varying the reaction time and temperature. The obtained wurtzite ZnS nanobelts grown at 180 ℃ over 6 h have shown different optical properties compared to the $ZnS(en)_{0.5}$ nanostructures, indicating their potential applications in nano-optoelectronic devices.

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Facile Self-Assembly Fabrication and Time-Resolved Fluorescence Study of Hybrid Au@P3HT Nanowires

이동기 장두전*

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Hybrid nanocomposites of conjugated polymers and inorganic nanocrystals have received intense attention for applications in optoelectronic devices such as light-emitting diodes, biosensors, and photovoltaic cells. In particular, one-dimensional nanostructures of conjugated polymers within hybrid nanocomposites, which possess advantages such as an efficient donor/acceptor interface, phase separation at the nanometer scale, and one-dimensional anisotropy that allows the photochemical generation of spatially separated charge carriers and the supply of a quick route for carrier transportation to the electrode, are expected to have improved efficiency in organic photovoltaic devices. Thus, we have fabricated facilely hybrid poly(3-hexylthiophene) (P3HT)-coated gold (Au@P3HT) nanowires via a self-assembly approach of Au@P3HT nanocomposites in poor solvents such as cyclohexanone. The morphology of produced hybrid Au@P3HT nanowires has been studied by transmission electron microscopy and scanning electron microscopy images. The dynamics of photo-generated excitons in hybrid Au@P3HT nanowires has also been investigated in comparison with that in Au@P3HT nanocomposites using a time-resolved fluorescence spectroscopy, revealing that the first-excited singlet-state decay of hybrid Au@P3HT nanowires is found to be slower than that of Au@P3HT nanocomposites due to conformational effects of one-dimensional nanostructures.

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Catalytic performances of silica-coated Ag/Au alloy nanoboxes synthesized via galvanic replacement

이재원 장두전*

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Nanoscale noble-metals have attracted attention from researchers in various fields of study because of their unusual optical properties as well as novel chemical properties. It is well-known that nanoparticles of noble-metals show strong absorption bands in the visible region due to their surface-plasmon oscillation modes of conductive electrons. Silver nanocubes stand out from various types of Silver nanostructures due to their superior performance in a range of applications involving localized surface plasmon resonance, surface-enhanced Raman scattering, and biosensing. In addition, extensive efforts have been devoted to the investigation of Gold-based nanocomposites to achieve high catalytic performances and utilization efficiencies. Silica-coated Ag/Au composite hollow nanoboxes having high catalytic performances and enhanced catalytic reusability have been fabricated via a galvanic replacement reaction of silica-coated silver nanocubes. Compared with silica-coated Ag nanocubes, silica-coated Ag/Au composite nanoboxes have been found to catalyze the degradation of 4-nitrophenol more rapidly in the presence of $NaBH_4$ due to fast diffusion. In contrast to bare Ag/Au composite nanoboxes, silica-coated Ag/Au composite nanoboxes can be recycled continuously for the catalytic degradation of 4-nitrophenol in the presence of $NaBH_4$. We consider that silica coating enhances the stability of Ag/Au composite nanoboxes enormously by blocking the dissolution and aggregation of nanoparticles thoroughly.

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Synthesis of Composition-Gradient Cd1-xZnxS Quantum Dots by Facile Cation Exchange to Controlled Their Optical Properties

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서울대학교 화학부

A new method is reported to synthesize water-soluble Cd1-xZnxS alloy quantum dots (QDs) having chemical-composition gradient (G?Cd1-xZnxS). The gradient in composition has been achieved by cation exchange of Zn2+ from Cd2+ in as-prepared CdS QDs. Due to the difference of solubility product constant (Ksp, at 25°C) between CdS and ZnS nanocrystals, the G?Cd1-xZnxS QDs consist of Cd-rich inner cores and Zn-rich outer shell. By controlling the ratios of [Zn] to [Cd], composition variable G?Cd1-xZnxS QDs (x = 0.13~0.92) have been synthesized. The wide range of emission wavelength (477 - 510 nm) is obtained without changing the crystal size. Due to the shell effect of ZnS, the as-prepared G?Cd1-xZnxS QDs possess higher QY and longer lifetime than CdS QDs. Also, we have compared the impact of inner structure on their optical properties by comparing 4 types of QDs: CdS, G?Cd1-xZnxS, CdS@ZnS core-shell (C?Cd1-xZnxS), homogeneous Cd1-xZnxS alloy (H?Cd1-xZnxS) QDs. These QDs have similar size and composition. We demonstrate the impact of the inner structure on the carrier relaxation of Cd1-xZnxS alloyed QDs. Lifetime and QY has been used to estimate the values of the radiative relaxation rate and nonradiative relaxation rate. There are several nonradiative relaxation processes including carrier trapping at QD defect states or surface states, quenching processes due to the QDs local environment, relaxation from the trap states, and so on. Results show that the G?Cd1-xZnxS QDs has the longest lifetime due to surface passivation with minimized lattice mismatch.

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Laser-induced fabrication of hollow platinum nanospheres to have enhanced catalytic performances

이혜리 장두전*

서울대학교 화학부

Enhanced catalytic performances of a nanocatalyst have been observed to irradiation of a pulsed Nd:YAG laser at 355 nm to platinum particles of less than 150 nm in aqueous solution. The connected hollow platinum nanospheres were successfully synthesized by laser treatment without any linkers. Nanosecond laser-induced heating has been employed to melt the surface of the platinum nanostructures, giving rise to connecting each other due to the thermalized photon energy of platinum-plasmon resonances. For this purpose two types of nanocatalysts; hollow platinum nanospheres and laser-treated hollow platinum nanospheres were prepared in this study. Catalytic activity of platinum nanospheres was tested for the reduction of rhodamine B in the presence of potassium borohydride. The reaction rate is the pseudo-first-order with respect to rhodamine B. From the average reaction rate constants at different temperatures, we determined the activation energy, the entropy of activation, and the pre-exponential factor for each type of platinum nanostructure. The kinetic data indicate that the laser-treated platinum nanopspheres are catalytically more active than hollow platinum nanospheres. All data obtained for t_0, which a certain period of time was required for the rhodamine B to absorb onto the catalyst's surface before the reaction could be initiated. Therefore, we consider that an induction time related to the surface reaction.

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Non-Hamiltonian approach for simulating the nonadiabatic dynamics

김현우 이영민*

포항공과대학교 화학과

Nonadiabatic transitions are often involved in important biological phenomena such as electron, proton, and excitation energy transfer processes. In theoretical chemistry, various semiclassical approaches have been proposed for understanding nonadiabatic dynamics. However, they always involve approximations that may limit their applicabilities. For example, semiclassical dynamics with Poisson bracket mapping equation (PBME) shows reliable results only for short-time simulations. Here, to improve PBME dynamics, we present its non-Hamiltonian variant by recovering the effect of approximated terms. We demonstrate that this non-Hamiltonian PBME performs well for explaining nonadiabatic dynamics in the spin-boson model. Because this simple model is also related to more sophisticated charge transfer reactions, we expect that non-Hamiltonian PBME can be applied to performing nonadiabatic simulations of such systems.

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Active role of a water molecule in pH dependent behavior of the bioluminescent luciferase

김현우 이영민*

포항공과대학교 화학과

While bioluminescence is widely applied in various imaging techniques, understanding on its detailed mechanism is still limited. For instance, the role of the protein in the luminescent process is not clearly explained yet. In fact, the protein can play an essential role in pH responses of bioluminescent systems because proteins usually contain considerable number of titratable residues. In this poster, we account for pH dependent behavior of a bioluminescent luciferase-oxyluciferin system by employing molecular dynamics (MD) simulations and quantum mechanical / molecular mechanical (QM/MM) calculations. We reproduce red-shifted emissions in acidic conditions as consistent with previous experimental and theoretical reports. More importantly, we observe that a water molecule inside the active pocket can enhance flexible motions of neighboring molecules. These flexibly wandering charged molecules effectively cancel the pH dependent emission changes. With this, we suggest that the active pocket in the luciferase remains dry during the bioluminescent process.

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Study on the fabrication of TFT type gas sensor based on polyaniline

주동우 황기환 부진효*

성균관대학교 화학과

Recently, importance of gas sensor is on the rise which make we get the response signal rapidly when it detect the toxic gas.generally performance of gas sensor is decided by the sensitivity, selectivity and stability about the target gas.PANI is an excellent material for ammonia sensing as it deprotonates the amine groups in the emeraldine salt converting it to the emeraldine base form with a corresponding drop in conductivity of several orders of magnitude.In this study, we synthesized the polyaniline emeraldine base which is conducting polymer. And we fabricated the thin film with it. Then performed the experience about ammonia gas sensing.In detail, we mixed the polyaniline emeraldine base powder, dodecyl benzensulfonic acid(DBSA) and chloroform. And then we fabricated the polyaniline emeraldine base thin film with the mixed solution by spin coating technique.We characterizated the thickness and morphology of thin film by SEM and we used XRD to characterizate the crystallinity of thin film.Also we characterizated the sheet resistance and signal of ammonia gas by four probe point and keithley 2400 respectively.

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Solvolysis of 5-dimethylamino-naphthalene-1-sulfonyl chloride

고한중

전주교육대학교 과학교육과

The solvolysis rate constants of 5-dimethylamino-naphthalene-1-sulfonyl chloride in 31 different solvents are well correlated with the extended Grunwald-Winstein equation, using the NT solvent nucleophilicity scale and YCl solvent ionizing scale, with sensitivity values of 0.96±0.09 and 0.53±0.03 for l and m, respectively. These l and m values can be considered to support a SN2 reaction pathway having somewhat similar transition state (TS) structure with that of the benzenesulfonyl chloride reaction, in which the bond formation is ahead of the bond breaking on the bases of the magnitudes of l (0.96) and m (0.53). This interpretation is further supported by the solvent kinetic isotope effects (SKIE, 1.34 to 1.88). Also, the selectivity values (S = 1.2 to 2.9) obtained in binary solvents were consistent with the proposed mechanism.

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Study of bound Rydberg states of HeH by using multichannel quantum defect theory (MQDT)

이천우

아주대학교 화학과

HeH 분자의 Rydberg state 들에 대한 스펙트럼은 Ketterle 에 의해 실험적으로 철저한 분석이 이루어져 있다. 이 분자에 대한 quantum defect 곡선은 Rydberg basis 함수로서 Kaufemann basis 함수를 이용하여 *n*sσ, *n*pσ, *n*pπ, *n*dπ series 들에 대해 multi-reference configuration interaction (MRCI) 방법으로 계산을 하였다. 이들 quantum defect 곡선을 이용하여 HeH 의 bound state 에너지를 multichannel quantum defect theory (MQDT) 를 이용하여 계산한 결과를 발표하고자 한다.

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Multichannel quantum defect (MQDT) study of effects of interloper 2p2p $^1\Pi_u$and $^1\Sigma_u$ series on the vib-rotational levels of $^1\Pi_u$ states using the quantum defect curves obtained by multi-reference configuration interaction (MRCI) method

이천우

아주대학교 화학과

Multi-reference configuration interaction (MRCI) method 을 이용하여 계산한 quantum defect 곡선을 이용하여 Multichannel quantum defect theory (MQDT) 를 써서 리튬 dimer 의 $^1\Pi_u$ states 들에서 보이는 2p2p $^1\Pi_u$ interloper 에 의한 영향을 조사하였다. 또한 C, D $^1\Pi_u$ 의 vib-rotational level 들의 인접 $^1\Sigma_u$ 와의 상호작용에 의한 perturbation 역시 MQDT 이론을 이용하여 조사하였다.

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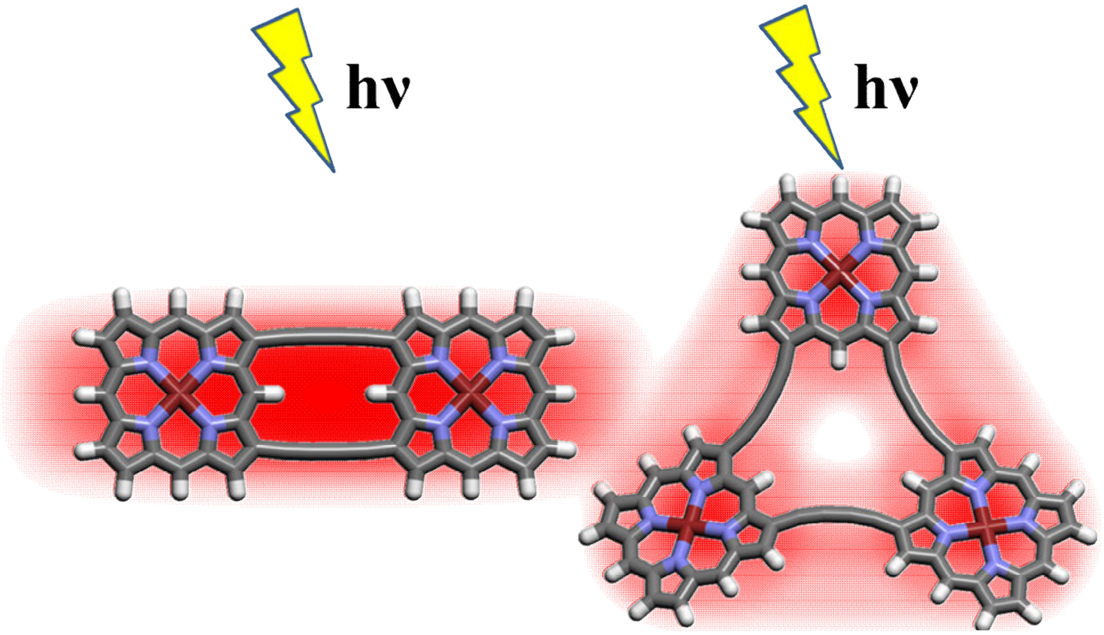
Excited-state electronic couplings in 1,3-butadiyne-bridged Zn(II)porphyrin dimer and trimer

이상수 김동호*

연세대학교 화학과

Recently, many research groups have made strenuous efforts toward the development of π-conjugated molecular systems, which may be utilized as functional soft materials and molecular-level devices for advanced technological functions. In particular, conjugated porphyrin oligomers have been one of the most extensively studied molecular motifs in light of their high stabilities, strong electronic absorptions in the visible region, emissive properties of certain porphyrins, efficient energy and electron transfer reactions, nonlinear optical properties, and easily tunable optical properties. In this work, we have comparatively investigated the electronic couplings in 1,3-butadiyne-bridged Zn(II) porphyrin dimer D and trimer T by measuring their excited-state properties at ensemble and single molecular levels. The porphyrin moieties are connected by two 1,3-butadiyne bridges via β-to-β connection to form a rectangular and a triangular shape for D and T, respectively. Based on various ensemble and single molecular experiment results, it was suggested that while single chromophore-like, strongly interacting behaviors have been revealed for D, the coupling in T has been indicated to be not so strong. In conclusion, our study demonstrates that butadiyne linkages play a specific role in the electronic communication in porphyrin oligomers. We think that this study will be a guideline for further investigations on the strongly coupled systems in other molecular arrays for future applications as photonic devices.


hν
hν

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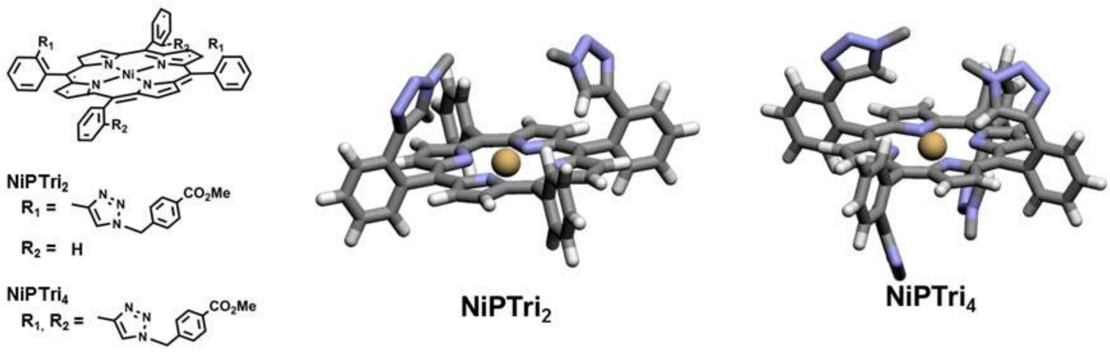
Modification of Axial Coordination in Nickel(II) Porphyrins by Functional Triazole Substituents

오주원 김동호*

연세대학교 화학과

The coordination of ligand to transition metal compound is influenced by the internal and external environment. Among those metal compounds, Ni(II) porphyrins display distinctive excited-state coordination processes where both dissociative and associative coordination reactions take place upon photoexcitation. It is, therefore, of great interest to see which factors affect the coordination chemistry of nickel porphyrins. In this regard, it is quite relevant to explore an introduction of functional substituents to Ni(II) porphyrins for their coordination control at molecular level. Based on this concept, we have designed novel functional Ni(II) porphyrins containing two and four triazole groups at the ortho-position of each phenyl group, which are denoted as NiPTri2 and NiPTri4, respectively.We have performed a comparative analysis of the effect of functional substituents on photoinduced ligation and deligation processes of NiPTri2 and NiPTri4 between neutral (i.e., pyridine) and anionic ligand (i.e., cyanide), by spectroscopic titration method and femtosecond time-resolved transient absorption spectroscopy.In this study, we have revealed the effective molecular control of ligation processes by triazole substituents on the porphyrin periphery depending on the type of ligand. Our findings presented here will provide a useful guideline on the coordination of metalloporphyrin containing functional substituents.


R$_1$
R$_2$
R$_1$
Ni
N
N
N
N
R$_2$
NiPTri$_2$
R$_1$ =
N
N
N
CO$_2$Me
R$_2$ = H
NiPTri$_4$
R$_1$, R$_2$ =
N
N
N
CO$_2$Me
NiPTri$_2$
NiPTri$_4$

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In silico study for the chemical reactivity of anionic metal clusters

임은학 김성근*

서울대학교 화학부

Metals that are normally inert can be activated when placed at a different oxidation state. Injecting an electron is a straightforward way to change the oxidation state of a metallic system, which may affect its chemical reactivity toward its adsorbate. We carried out DFT calculations for anionic metal clusters having a size much smaller than nano particles to investigate their chemical reactivity. We examined the charge distribution within the metal clusters, the change in the adsorbate structure, and the interaction between the anionic metal clusters and the adsorbate, which suggests a certain set of optimal conditions for the activation of anionic metal system.

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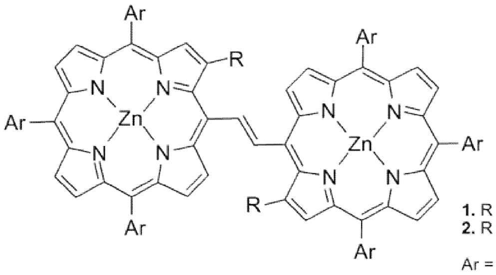
Control of the Conformational Dynamics of *meso-meso* Vinylene-bridgedZn(II) porphyrin Dimers through Diamine Coordination

손민정 김동호*

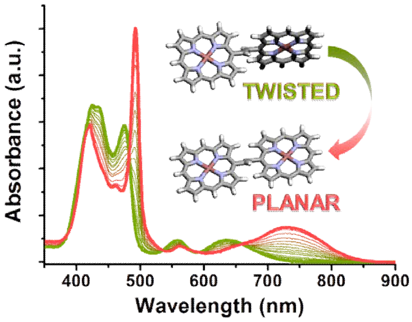
연세대학교 화학과

Unraveling the dynamics of conformational alteration in double-bond linked π-conjugated systems has drawn attraction over decades, stemming from the spectroscopic studies on the *cis-trans* photoisomerization of stilbene. Herein, we have focused on controlling the rotational dynamics around the double bond bridges in two *meso-meso* vinylene-linked Zn(II) porphyrin dimers 1 and 2 (Figure) by using steady-state and time-resolved spectroscopy. In particular, we have attempted to manipulate the dihedral angles between the two porphyrin moieties systematically by introducing bidentate ligands of varying carbon chain lengths, α,ω-diaminoalkanes (*n*DA, n = 3, 4, 5, …, 10, 12). Both 1 and 2 showed very broad and structureless fluorescence emission with extremely large Stokes shift, implying the flexibility of the vinylene bridge, leading to numerous conformers with a range of dihedral angles between the two porphyrin rings. The time-resolved fluorescence profiles exhibited fast decay components when monitored at shorter wavelengths and corresponding rise components at longer wavelengths. For an elaborate control of the dihedral angles in ambient condition, 1 and 2 were titrated with *n*DA and different trends were observed depending on the length of the ligands. For 7DA complexes, the lower-energy Soret absorption bands were greatly sharpened and red-shifted with significant increase in intensity, and the Q bands were also prominently red-shifted. The fluorescence spectra were also red-shifted to the infrared region and the Stokes shifts were gradually decreased in all species upon coordination, converging to the smallest values observed for 7DA complexes, indicating that the dihedral angles are confined to a certain extent.



1. R = H
2. R = 3,5-dimethylphenyl

Ar = 3,5-di-*tert*-butylphenyl



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Spectroscopic Observation of Jet-cooled 2,5-Dichlorobenzyl Radical Generated by Corona Discharge

이은혜 윤영욱 이상국*

부산대학교 화학과

Transient species such as molecular ions and radicals have long believed to play an important role as reactionintermediates in chemical reaction. Vibronically excited but jet-cooled benzyl-type radical was generated by the corona discharge of precursor 2,5-dichlorotoluene seed on a large amount of inert carrier gas He using a pinhole-type glass nozzle, from which the vibronic emission spectra were observed with a long-path monochromator in the visible region. The radical was generated by dissociation of one of the methyl C-H bonds of precursor with a collision of metastable He. From an analysis of the visible emission spectrum observed, we found the evidence of the formation of the 2,5-dichlorobenzyl radical. The electronic energy in the $D_1 \rightarrow D_0$ transition and the vibrational mode frequencies of the 2,5-dichloronezyl radical in the D_0 state were accurately determined by comparison with ad initio calculations and the known vibrational data of the precursor. Furthermore, our results provide interesting information regarding the substituent effect on electronic transition energy.

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Distinct Role of Preferential Hydration in Protein Aggregation

정성호 함시현*

숙명여자대학교 화학과

Understanding the molecular determinants of the relative propensity for proteins to aggregate in a cellular environment is a central issue for treating protein-aggregation diseases and developing peptide-based therapeutics. Despite the expectation that protein aggregation can largely be attributed to direct protein-protein interactions within an aggregate or in solution, we here unveil a crucial role of hydration water in ruling the aggregation propensity of proteins both in vitro and in vivo. The overall protein hydrophobicity, defined solely by the hydration free energy of a protein in its monomeric state sampling its equilibrium structures, was shown to predominantly dictate the protein aggregation propensity in aqueous solutions. Striking discrimination of positively and negatively charged residues by the hydration water was also found. This effect depends on the protein net charge and plays a crucial role in regulating the solubility of the protein. These results pave the way for the design of aggregation-resistant proteins as biotherapeutics.

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Vibrational Spectroscopy and Dynamics of the Hydrazoic Acid in AOT Reverse Micelles

이주용 이경구[1] 곽경원[2] 조민행*

고려대학교 화학과 [1]군산대학교 화학과 [2]중앙대학교 화학과

IR probes have been extensively used to monitor local electrostatic and solvation dynamics. Particularly, their vibrational frequencies are highly sensitive to local solvent electric field around an IR probe. Here, we show that the experimentally measured vibrational frequency shifts can be inversely used to determine local electric potential and field distributions and solute-solvent electrostatic interaction energy. In addition, the upper limits of their fluctuation amplitudes are estimated by using the vibrational bandwidths. Applying this method to a core/shell model has often been used to describe water confined to the interior of reverse micelles.

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Nanometer-Scale Reverse Micelles Studied by FTIR Spevctroscopy and MD Simulation

김민석 이주용 조민행*

고려대학교 화학과

The properties of N-methylacetamide (NMA) molecules encapsulated in the reverse micelles (RM) formed by anionic surfactant aerosol OT (AOT), are studied with vibrational spectroscopy and computation. Vibrational spectra of the amide I' mode of the fully deuterated NMA-d_7 show gradual increase of peak frequencies and line broadening as the size of RM decreases. Analyses of the spectral features reveal the presence of three states of NMA-d_7 that correspond to NMA located in the core of water phase (absorption frequency of 1606 cm^{-1}) and two types of interfacial NMA near the surfactant layer (1620 and 1644 cm^{-1}). In larger RM's with water content w0=[D_2O]/[AOT]≥10, only the first two states are observed, whereas in smaller RM, the population of the third state grows up to 25% at w_0=2. These results indicate the general validity of the two-state core/shell model for the confined aqueous solution of NMA, with small modifications due to the system-dependent solute-interface interaction. However, simulations of small RM systems with $w_0 \leq 15$ show continuous variations of the population, frequency shifts and the solute-solvent interaction strengths at solute-interface distance less than 4 ?. Thus, the distinction of solute core/shell states tends to be blurred in small RM's but is still effective in interpreting the average spectroscopic observables.

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Fabrication of vertical silicon microwire arrays for enhanced light trapping using Deep Reactive Ion Etching

황인찬 엄한돈 서관용[1,*]

울산과학기술대학교(UNIST) 에너지공학과 [1]울산과학기술대학교(UNIST) 친환경에너지공학부

Silicon microwire array is one of the promising platforms as a means for developing highly efficient solar cells thanks to the enhanced light trapping efficiency. Among the various fabrication methods of microstructures, Deep Reactive Ion Etching (DRIE) process has been extensively used. In this presentation, we show precisely controlled vertical Si microwire arrays by tuning the DRIE process conditions. A periodic microdisks were patterned on 4 inch Si wafer (p-type, 1-10 Ωcm) using photolithography. After developing the pattern, 150-nm-thick Al was deposited and lifted-off to leave Al microdisk arrays on the starting Si wafer. Periodic Al microdisk arrays (diameter of 2 μm and periodic distance of 2 μm) were used as an etch mask. A DRIE process (Tegal 200) is used for anisotropic deep silicon etching. During the process, SF_6 and C_4F_8 gases were used for the etching and surface passivation, respectively. The length and shape of microwire arrays were controlled by etching time and SF_6/C_4F_8 ratio. After DRIE process, the residual polymer and etching damage on the surface of the microwires were removed using piranha solution followed by thermal oxidation (1000 °C, 3 hour). The oxide layer formed through the thermal oxidation was etched by diluted hydrofluoric acid (1 wt% HF). The surface morphology of a Si microwire arrays was characterized by field-emission scanning electron microscopy (FE-SEM, Hitachi S-4800). Optical reflection measurements were performed over 300-1100 nm wavelengths using a UV-Vis/NIR spectrophotometer (Cary 5000, Agilent). The total reflection by the microwire arrays sample was reduced from 20 % to 10 % of the incident light over the visible region when the length of the microwire was increased from 10 μm to 40 μm.

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Computational Studies on the Design of New Catalysts for Water Oxidation

Adhikary Keshab Kumar 김찬경*

인하대학교 화학과

Green plants convert carbon dioxide to sugar for energy storage via photosynthesis. From the mimicking more simple isolated process can be feasible to store the abundant solar energy as a renewable source. Hydrogen produced by using sun-light to split water into its elements has long been recognized as an ideal source of fuel. A free-standing PEC combined with a photosensitizer of metal molecular complex is a promising characteristic device to achieve water oxidation catalysis without application of any external bias. Iso-structural cubane-shaped catalysts or others with different ligands might be able to oxidize water under dark and illuminated conditions, where the primary step of photo-induced electron transfer obeys the Hammett linear free energy relationship. Some manganese clusters and many other clusters with high valance states have a promising key feature similar to the most important catalysts in nature, the water oxidizing complex of photosystem-II. We have performed computational modelling studies on these compounds.

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Theoretical Studies on the Bimolecular Nucleophilic Substitution Reactions for Y-substituted Phenoxy Hydrogen Isothiocyanophosphonate

Adhikary Keshab Kumar 김찬경*

인하대학교 화학과

The kinetics and mechanism of the pyridinolysis (XC5H4N) of phenoxy hydrogen isothiocyanophosphonate (Y-C6H4O(P=O)(H)NCS) in acetonitrile are investigated at room temperature 25.0oC. Physical and thermodynamic parameters as well as molecular orbital overlapping indicate the back-side nucleophilic attack of pyridines and leaving group (?NCS) departure strategies. According to the literature and several experimental evidences, concerted or a stepwise mechanistic route during the expulsion of isothiocyanate (NCS) leaving group from the intermediate or TS are possible, where positive and negative ρX, and βX values imply the characteristics of the nucleophilic attack. In addition, the steric effects of the ligands can play an important role in determining the rates of the reactions.

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Proline catalyzed Transamidation of amides: DFT study

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L-proline is known to catalyze the transamidation reaction between carboxamides and amines. The role of the catalyst was studied theoretically with the B3LYP//6-31++g* level of theory using Gaussian 09 package. The transamidation reaction without catalyst requires a higher barrier of 47.89 kcal/mol. In the presence of catalyst, however, the reaction proceeds through a multi-step mechanism and the energy barrier is much lower than the reaction without catalyst. We also studied the reaction mechanism in solvent, higher temperature, and the role of bulky groups in the real system. From this study, novel mechanism for dehydration is also proposed.

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Bifunctional Catalysts on desymmetrization reaction of anhydrides: ONIOM study

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The reaction between anhydride and methanol catalyzed by bifunctional Bronsted acid/base organocatalyst was investigated theoretically by ONIOM method. Calculations indicate that the energy barrier is quite high without catalyst, i.e. 30.8 kcal/mol. In the presence of catalyst, the reaction proceeds through a 2-step mechanism an energy barrier of 19.0 kcal/mol and 0.9 kcal/mol. The pyridine moiety works as a Bronsted base to activate methanol substrate, and the N atom attached to P atom as a Bronsted acid to activate the anhydride by hydrogen bonding. The role of enantioselectivity of the catalyst is consistent with experiment results.

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HF studies on the reaction mechanism of etherification catalyzed by AuCl3

매방 김찬경[1,*]

인하대학교 물리화학부/화학과 [1]인하대학교 화학과

The mechanism of etherification of alcohols catalyzed by AuCl3 was studied using the Hartree-Fock method with Gaussian program. Lanl2dz basis set was used for Au atom, 6-31G(d) for other atoms. The results shows that AuCl3 acts as a Lewis acid, coordinating with one alcohol molecule, which is then attacked by another alcohol acting as a nucleophile. We also studied the reaction mechanism in the absence of the catalyst. The PES of the catalytic cycles and the role of catalyst will be discussed in detail.

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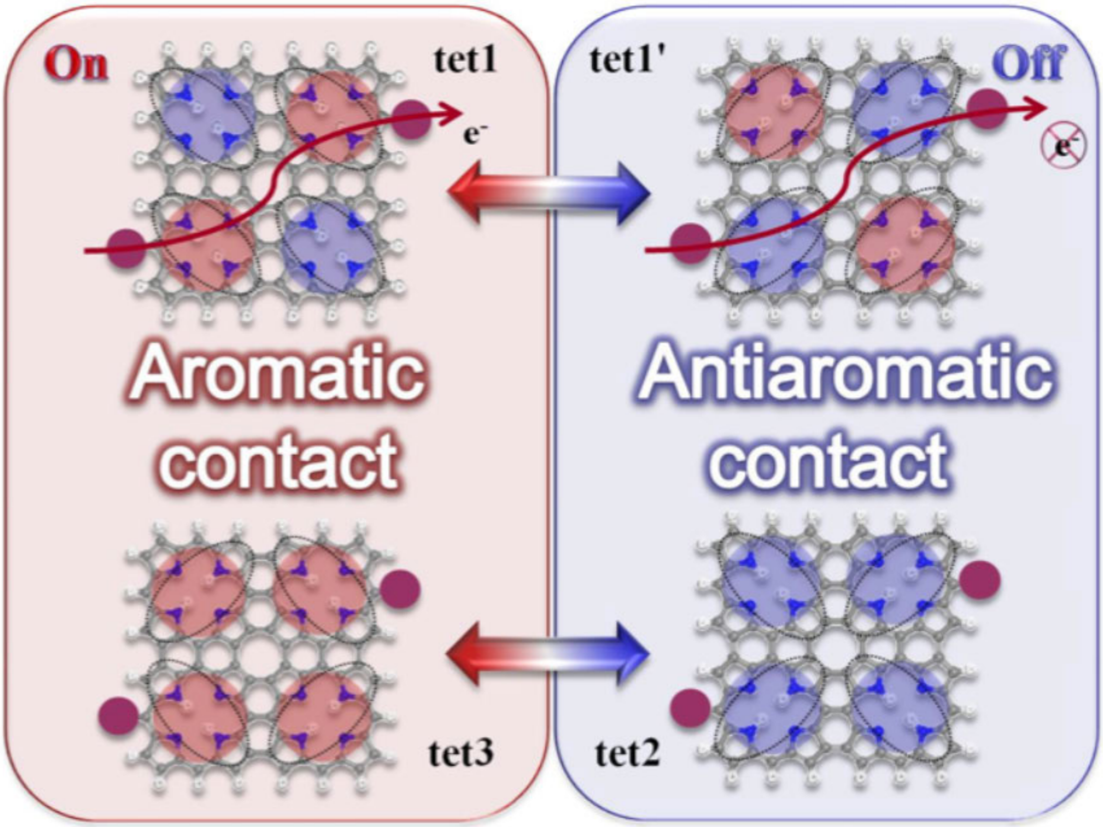
The Role of Aromaticity and the p-Conjugated Framework in Multiporphyrinic Systems as Single-Molecule Switches

최은영 박지현 이상욱*

울산대학교 화학과

A systematic analysis of electron-transport characteristics for monomer, dimer, and tetramer multiporphyrinic systems is presented, to provide a thorough understanding of the structural dependence of electron transport related to the aromatic nature of the contact structure. Theoretical inves- tigation shows that the electron-transport characteristics can be controlled by manipulating the p-conjugated framework in the multiporphyrinic systems through the arrangement of the inner hydrogen atoms. The designed p-conjugated framework assigns the distinct aromaticity on the contact structure, and the large aromatic nature of the contact structure increases conductivity. The feature emerging from this study is that the aromaticity and p-conjugated framework are important factors that control the electron-transport characteristics in molecular-scale electronic devices, such as single-molecule switches.


On
tet1
e⁻
tet1'
Off
e⁻
Aromatic contact
Antiaromatic contact
tet3
tet2

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Dependence of the four-atom reaction HBr + OH → Br + H2O on temperature between 20 and 2000 K

이종백[*] H. K. Shin[1] 김유항[2]

전남대학교 화학교육과 [1]Dept of Chem, Univ of nevada [2]한국과학기술한림원

A quasiclassical trajectory method is used to study the temperature dependence of the molecule-radical reaction HBr + OH → Br + H_2O over the range of 20 ? 2000 K. Potential energy surfaces are formulated with analytic forms of pair-wise additive two-body and nonadditive three-body interaction potentials. At temperatures above 300 K, the reaction occurs in *dir*ect collisions and the calculated rate constant fits the Arrhenius equation $k_{dir} = 1.11 \times 10^{-10} \exp(-796/T)$ $cm^3 molecule^{-1} s^{-1}$. At temperatures below 300 K, the reaction is attraction-driven and occurs through the formation of a collision-complex BrH…OH, which sufficiently long lived to enhance H-atom tunneling. A strong negative temperature dependence of the *com*plex-mode rate constant k_{com} is found between 20 and 300 K in consistent with the experimental data reported by various authors. The complex-mode rate constant fits $k_{com} = 1.43 \times 10^{-11} \exp(41/T)$ between 20 - 100 K and $k_{com} = 8.23 \times 10^{-12} \exp(104/T)$ between 100 - 300 K. At 20 K, $k_{comp} = 1.12 \times 10^{-10}$, which is nearly twice the direct-mode value at 1000 K.

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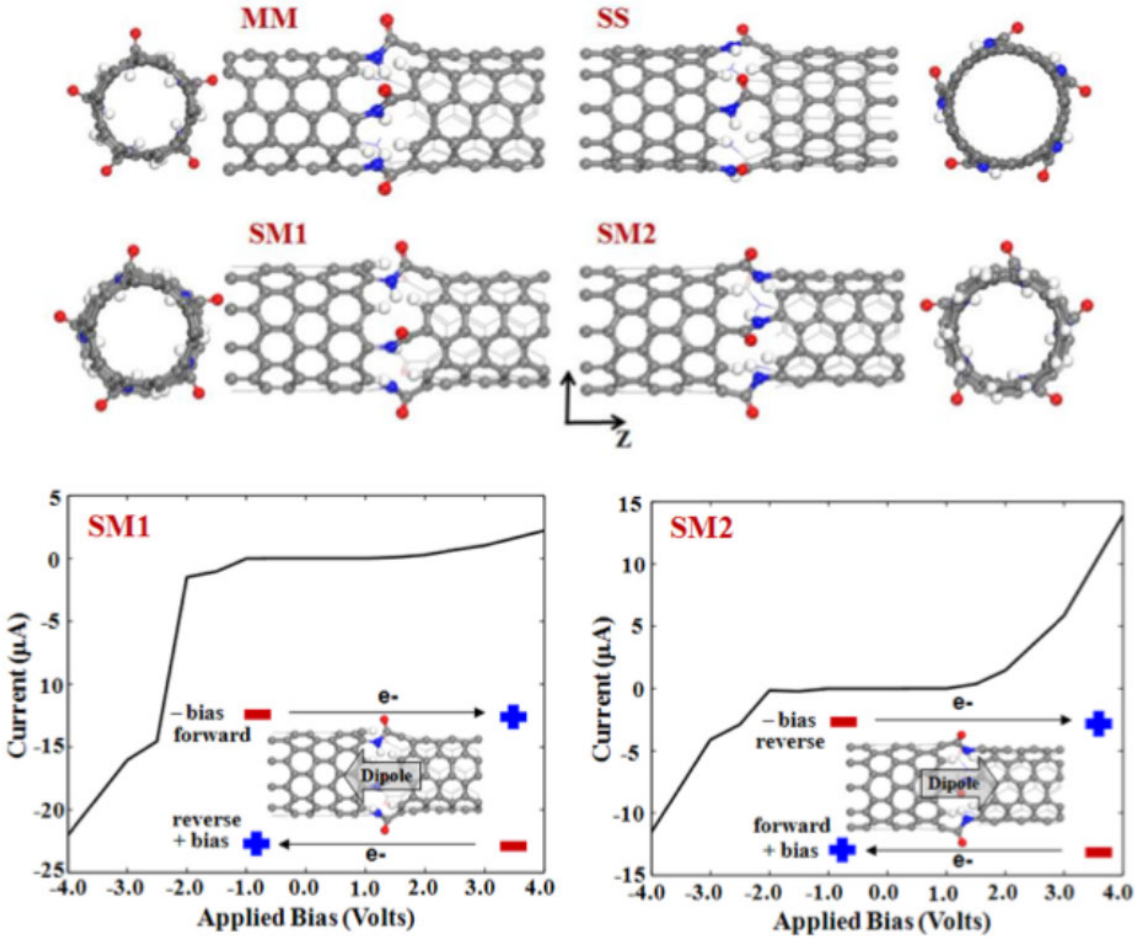
Electron transport through carbon nanotube intramolecular heterojunctions with peptide linkages

최은영 김민지 이상욱*

울산대학교 화학과

We present a systematic analysis of electron transport characteristics of carbon nanotube (CNT) intramolecular heterojunctions with peptide linkages, MM, SS, SM1, and SM2 where M and S stand for metallic and semiconducting CNT electrodes, respectively. Our theoretical investigations show that the incorporation of peptide linkages and their associated dipole moments play an important role in determining the electron transport characteristics and lead to materials with unique properties, such as Schottky-like behavior. Furthermore, we show that the Schottky-like behavior is observed in our SM1 junction but not in the SM2 junction because of the different effects that arise from both the direction and strength of their dipole moments. We believe that our results will pave the way towards the design and implementation of various electronic logic functions based on carbon nanotubes for applications in the field of nanoelectronics.



MM
SS
SM1
SM2
Z
SM1
Current (μA)
5
0
-5
10
-15
-20
-25
-4.0
-3.0
-2.0
-1.0
0.0
1.0
2.0
3.0
4.0
Applied Bias (Volts)
– bias
forward
e-
Dipole
reverse
+ bias
e-
SM2
Current (μA)
15
10
5
0
-5
-10
-15
-4.0
-3.0
-2.0
-1.0
0.0
1.0
2.0
3.0
4.0
Applied Bias (Volts)
– bias
reverse
e-
Dipole
forward
+ bias
e-

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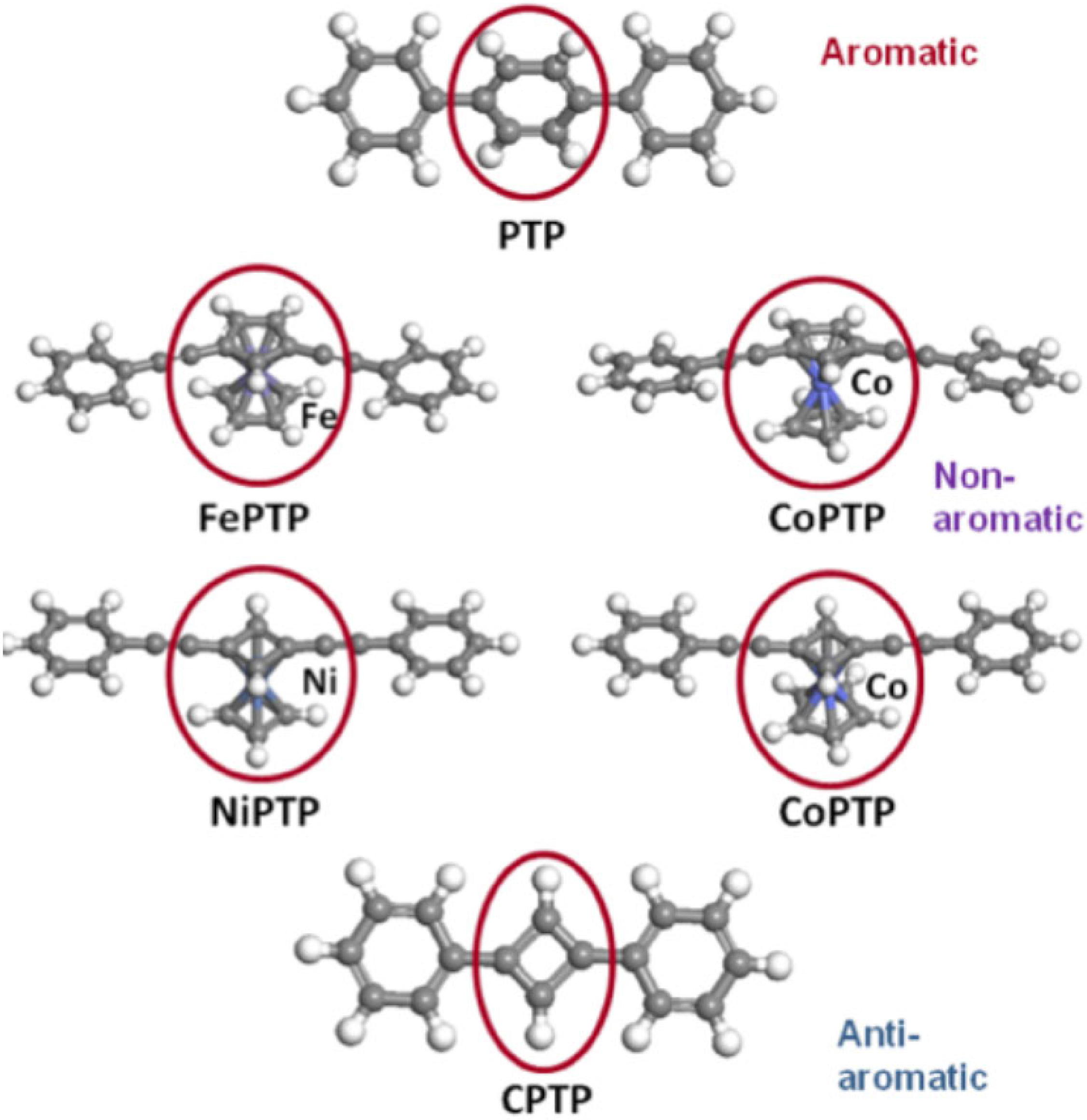
Control of Electron Transport by Manipulating the Conjugated Framework

최은영 김예진 이상욱*

울산대학교 화학과

We present a systematic analysis of molecular level alignments and electron transport characteristics based on the nonequilibrium Green's function (NEGF) approach combined with density functional theory (DFT) for six conjugated molecules (PTP, CPTP, NiPTP, CoPTP4, CoPTP5, and FePTP) containing different types of conjugated frameworks. The conjugated molecules are classified into three groups according to the incorporated component into the conjugated framework where group I, group II, and group III contain antiaromatic, nonaromatic, and aromatic units, respectively. The results show that the combining of non- and antiaromatic components increases the conductance due to the close alignment of the HOMO level relative to the Fermi level. Consequently, the order of current follows the manner of group I > group II > group III ([NiPTP > CoPTP4 > CPTP] > [CoPTP5 > FePTP] > [PTP]). The important feature emerging from this work is that the distinct response of each group to molecule-contact coupling and applied bias voltage causes distinguishable features of electron transport characteristics and these factors may give an insight into the design of new nanoscale molecular electronic devices.


Aromatic
PTP
Fe
FePTP
Co
CoPTP
Non-aromatic
Ni
NiPTP
Co
CoPTP
CPTP
Anti-aromatic

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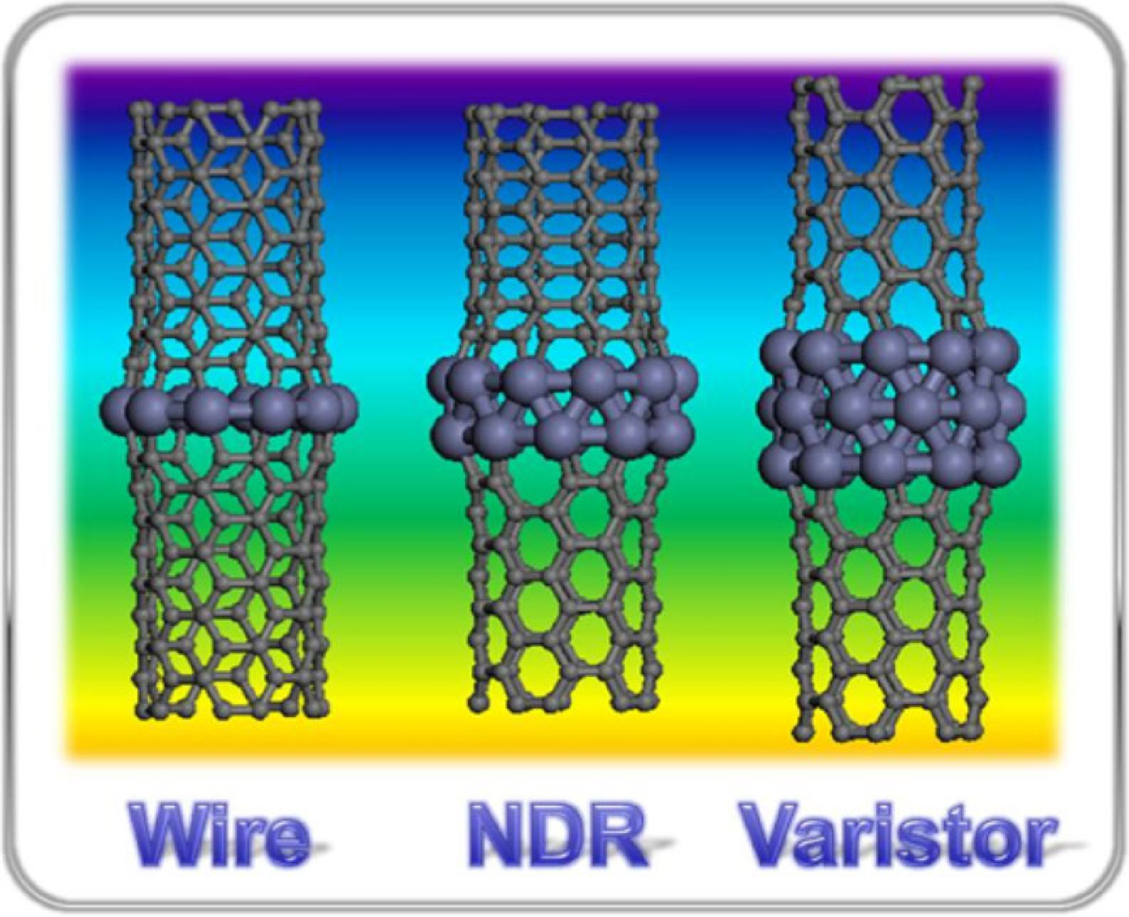
Designing Nanogadgets by Interconnecting Carbon Nanotubes with Zinc Layers

최은영 김태원 이상욱*

울산대학교 화학과

Using first-principles calculations we propose a new approach for the design of functional units obtained by interconnecting carbon nanotubes (CNTs) with different numbers of zinc layers. The theoretical investigations on electron transport properties of the resulting 1D heterojunctions containing CNTs with same or different chiralities (i.e., metallic or semiconducting) and one, two, or three zinc layers illustrate that the junctions with two semiconducting CNTs show semiconducting I-V characteristics while the junctions with two different CNT electrodes (metallic and semiconducting) show rectifying diode properties. The remarkable features emerging from this study is that the zinc layers behave as a momentum filter (near the Fermi energy the Bloch states having the same orbital character as the molecular states conduct well) when they are inserted within metallic CNT electrodes thereby providing 1D heterojunctions that can act as a wire-like, negative differential resistance (NDR), or varistor-type nanoscale device. Our results prove the idea that it is possible to design specific heterojunctions, which can select a conducting channel between two electrodes. Also, it is worth mentioning that in this study for the first time we have designed a nanoscale device with the characteristics of a varistor.


Wire
NDR
Varistor

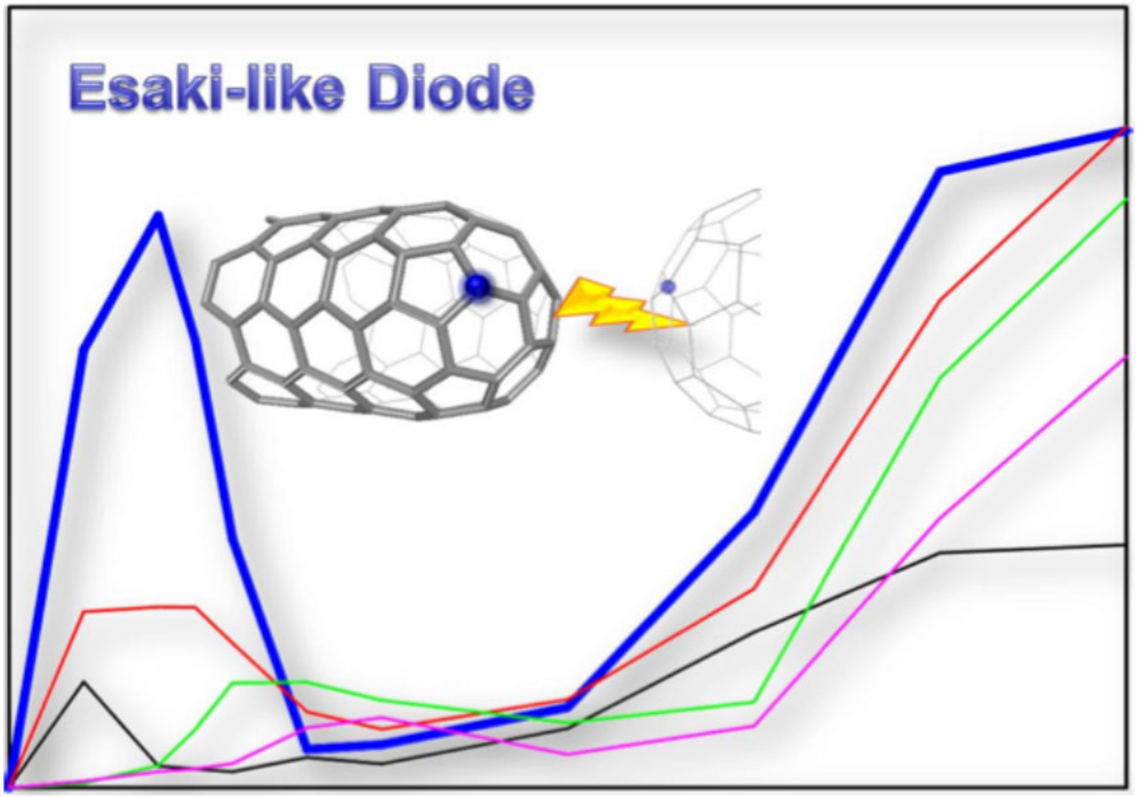
일시: 2014년 4월 16~18일(수~금) 3일간
장소: 일산KINTEX
발표코드: **PHYS.P-281**
발표분야: 물리화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Designing Nanogadgetry for Nanoelectronic Devices with Nitrogen-Doped Capped Carbon Nanotubes

최은영 홍정의 이상욱*

울산대학교 화학과

A systematic analysis of electron transport characteristics for 1D hetero- junctions with two nitrogen-doped (N-doped) capped carbon nanotubes (CNTs) facing one another at different conformations is presented con- sidering the chirality of CNTs (armchair(5,5) and zigzag(9,0)) and spatial arrangement of N-dopants. The results show that the modification of the molecular orbitals by the N-dopants generates a conducting channel in the designed CNT junctions, inducing a negative differential resistance (NDR) behavior, which is a characteristic feature of the Esaki-like diode, that is, tunneling diode. The NDR behavior significantly depends on the N-doping site and the facing conformations of the N-doped capped CNT junctions. Furthermore, a clear interpretation is presented for the NDR behavior by a rigid shift model of the HOMO- and LUMO-filtered energy levels in the left and right electrodes under the applied biases. These results give an insight into the design and implementation of various electronic logic functions based on CNTs for applications in the field of nanoelectronics.


Esaki-like Diode

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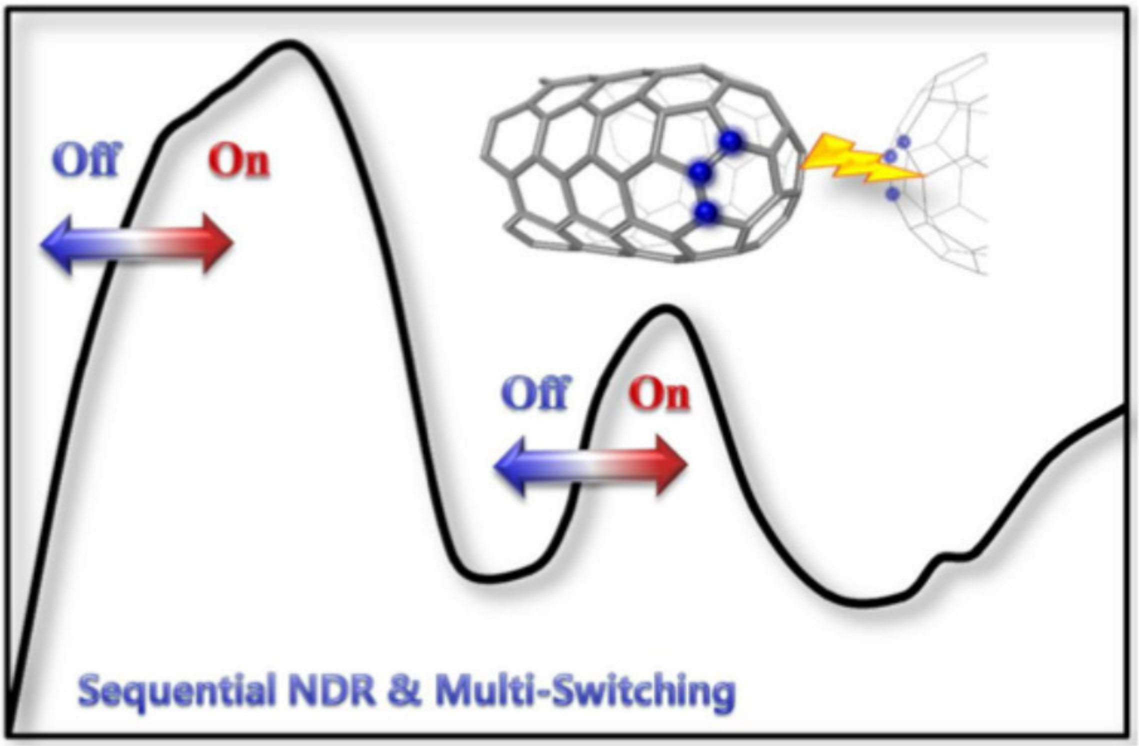
발표분야: 물리화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Electron transport characteristics of one-dimensional heterojunctions with multi-nitrogen-doped capped carbon nanotubes

최은영 오례경 이상욱*

울산대학교 화학과

We present a systematic analysis of electron transport characteristics for one-dimensional heterojunctions with two multi-nitrogen-doped (multi-N-doped) capped carbon nanotubes (CNTs) facing one another at different numbers of nitrogen atoms and conformations. Our results show that the modification of the molecular orbitals by the nitrogen dopants generates conducting channels in the designed heterojunctions inducing multi-switching behavior with sequential negative differential resistance (NDR). The NDR behavior significantly depends on the doping site and conformation of doped nitrogen atoms. Furthermore, we provide a clear interpretation for the NDR behavior by a rigid shift model of the HOMO- and LUMO-filtered energy levels in the left and right electrodes under the applied biases. We believe that our results will give an insight into the design and implementation of various electronic logic functions based on CNTs for applications in the field of nanoelectronics.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Sequential NDR & Multi-Switching

일시: 2014년 4월 16~18일(수~금) 3일간
장소: 일산KINTEX
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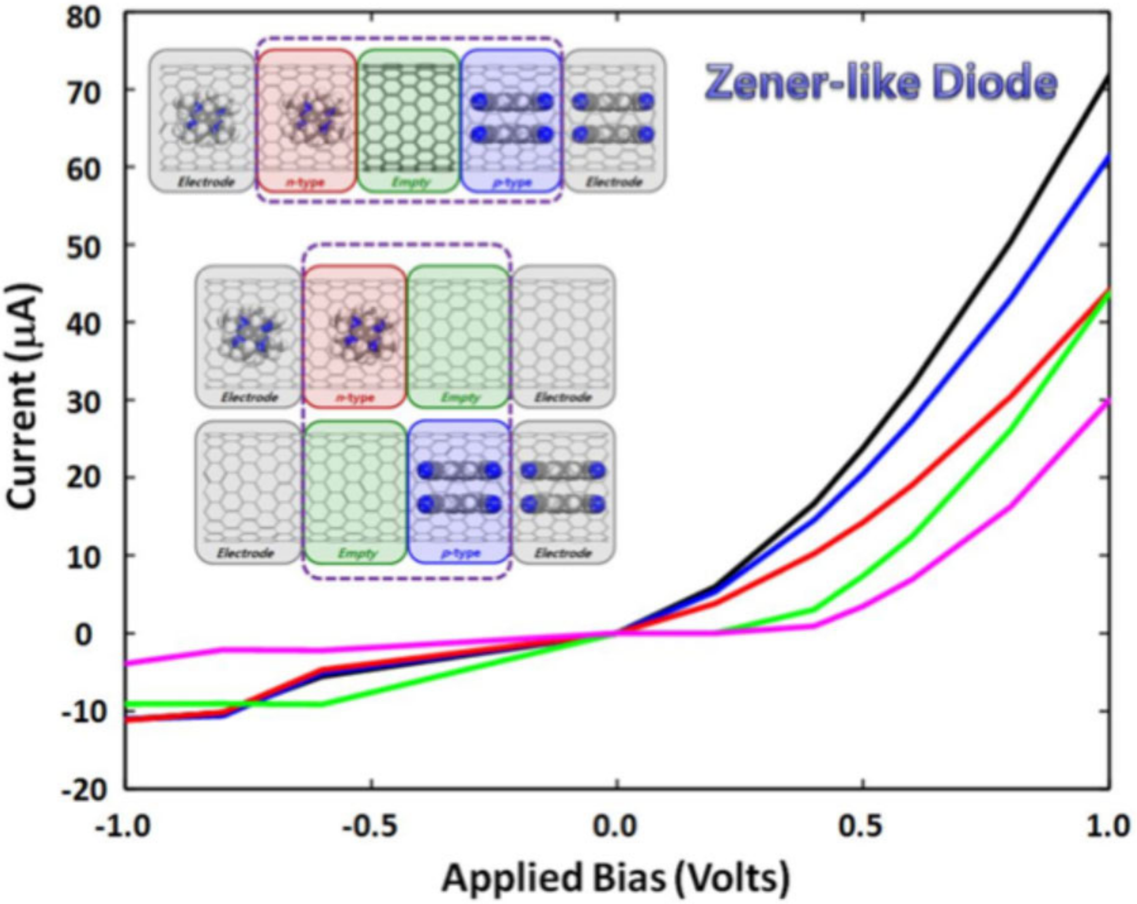
Electron transport characteristics of organic molecule encapsulated carbon nanotubes

최은영 조재호 이상욱*

울산대학교 화학과

One-dimensional carbon nanotube (CNT) junctions with interesting device characteristics have been designed by encapsulating p- and n-type organic molecules into CNTs with electrophilic tetracyano-p-quinodimethane (TCNQ) and nucleophilic tetrakis(dimethylamino)ethylene (TDAE) molecules in order to explore the effect of encapsulation of organic molecules and rectifying behaviors of the designed one-dimensional CNT p?n junctions. Our results show that p- and n-type doping of CNTs and their associated charge transfer play an important role in determining the electron transport characteristics and lead to materials with unique properties, p?n junction diode, i.e. Zener-like diode. Furthermore, we show that the operational device characteristics of non-covalently doped CNT junctions originate from the distinct response of intrinsic transmission peaks of pure CNTs according to the type of dopant and the applied bias. We believe that the results give an insight into the design and implementation of various electronic logic functions based on CNTs for applications in the field of nanoelectronics.



Zener-like Diode
Electrode
n-type
Empty
p-type
Electrode
Electrode
n-type
Empty
Electrode
Electrode
Empty
p-type
Electrode
Current (μA)
80
70
60
50
40
30
20
10
0
-10
-20
-1.0
-0.5
0.0
0.5
1.0
Applied Bias (Volts)

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발표종류: 포스터, 발표일시: 수 16:00~19:00

Stability of Morin in Aqueous Solution

박형련* 임서은 박옥현 박기민[1]

전남대학교 화학과 [1]경상대학교 화학교육과

Polyphenols have attracted considerable attention as agents that protect cells or molecules from oxidative myocardial injury last few decades. The flavanols are a family of naturally occurring polyphenols that are present in a wide variety of plant species. Morin (3,5,7,2',4'-pentahydroxyflavone) is one of flavonols and it is an important bioactive compound by interacting with nucleic acids, enzymes and protein. The aim of this study is to prove its stability in aqueous solution using spectroscopic methods. The substance is soluble in water and its absorption spectrum contains two maximum peaks at 263 nm and 387 nm. The absorption spectrum of 50 μM deaerated aqueous morin solution did not change, even if the solution was left in the dark at room temperature for 5 days. However, the absorption spectrum of the aerated aqueous morin solution did change as time passes. The absorption maximum peak at 387 nm is continuously shifted to longer wavelength when the storage time of the solution increased. Moreover, the absorption spectrum of morin is also changed continuously according to the pH values of the aqueous solution. The substance emits weak fluorescence with maximum peak at 515 nm. Its fluorescence spectrum is also changed according to the pH values in the solution. These results indicate that flavonoid morin is very unstable in aqueous solution. The reason of this can be explained by the oxidation of morin in aqueous solution.

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Preparation of hydrophobic PDMS-coating on mesoporous silica and their use as pre-concentrating agents of gas analytes

박은지 정명근 김영독*

성균관대학교 화학과

Mesoporous silica with a mean pore size of ~13 nm was coated by polydimethylsiloxane (PDMS) using a thermal deposition method. We show that inner-walls of pores larger than ~15 nm can be successfully coated by thin layers of PDMS, and surfaces consisting of the PDMS-coated silica showed superhydrophobic nature with a water contact angle close to 170^{o}. We used the PDMS-coated silica as adsorbents of various gas phase analytes, which are chemical warfare agent (CWA) simulants. PDMS-coated silica allows molecular desorption of various CWA simulants even after exposure under highly humid conditions, and therefore applicable as pre-centration agents of gas phase analytes, which can enhance sensitivity of various sensors.

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Dynamics of O_2 Rebinding to Myoglobin Probed by Time-resolved Vibrational Spectroscopy

박성철 박재홍 임만호*

부산대학교 화학과

Time-resolved vibrational spectroscopy was used to probe the rebinding dynamics of O_2 to myoglobin (Mb) in the time range from femtosecond to microsecond after excitation of oxymyoglobin (MbO_2) in D_2O with a 575nm pulse at 293K. Since the weak O-O stretch band is overlapped with the strong absorption bands in the 1300 ~ 1000 cm^{-1} region by water solvent, protein, and buffer molecule, difference time-resolved spectra ($Mb^{16}O_2$ - $Mb^{18}O_2$) were obtained to delineate O_2-related bands from the absorption changes due to conformational and thermal relaxation. The O-O stretch mode in MbO_2 is known to exhibit two conformational bands but one conformation band in $Mb^{16}O_2$ is split due to a perturbing vibration, resulting in three absorption bands for $Mb^{16}O_2$ (1147, 1123, and 1104 cm^{-1}) and two absorption bands for Mb18O_2 (1086 and 1067 cm^{-1}). Therefore, after the Q-band excitation the difference transient spectra exhibit three photo-bleaching bands for $Mb^{16}O_2$ and two transient absorptions for $Mb^{18}O_2$. All the transient signals decay with the same kinetics and were described by two exponential function plus an equation describing bimolecular reaction. The recovered time constants for the exponential function were 3 ps (75%) and 47 ns (14%) and the bimolecular rate constant was 24×10^6 M^{-1}s^{-1}. The 3 ps and 47 ns decays were attributed to thermal relaxation of six-coordinate heme subsequent to fast electronic relaxation without photodeligation and geminate recombination (GR) of O_2 after photodeligation, respectively. The cooling process for the six-coordinate heme group can be observed due to anharmonic coupling of low frequency modes with the O_2 stretching mode. When photoexcited in the Q-band, about 25% of MbO2 undergoes photodeligation (quantum yield, QY = 0.25), about 55% of the deligated O_2 geminately rebinds in a time constant of 47 ns, and the remaining O_2 escapes into solvent and bimolecularly rebinds with the rate constant of 21×10^6 M^{-1}s^{-1}. Fast and efficient GR of O_2 indicates that the heme pocket is efficient in trapping the deligated O_2. Conformation-independent dynamics of

photoexcited MbO_2 suggests that the O_2 binding characteristics is independent of conformatiomnal substates of MbO_2 or transition between conformational substates is faster than 47 ns.

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발표분야: 물리화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Structural Dynamics of C2H4I2 in Methanol: A QM/MM-MD Study

Manik Kumer Ghosh 최철호*

경북대학교 화학과

The photodissociation dynamics of iodine elimination reaction of 1,2-diiodoethane in methanol has been studied by applying QM/MM-MD simulations. Both ab initio quantum mechanical calculation and QM/MM-MD simulation has been applied for determining the rotational barrier of C2H4I2 molecule. Upon excitation of the molecule, C?I bond has been broken within 200 fs time scale and formed radical C2H4I (bridged or classical). The C ? I bond dissociation dynamics of gauche geometries are slower than the anti conformers of C2H4I because of steric hindrance. Radical C2H4I further bind with the free iodine and form stable complex C2H4I---I without any energy barrier. This complex could be mixture of bridged and classical species. Surrounding solvent structure of methanol is responsible for making stable C2H4I---I complex rather than comparatively less stable radical C2H4I + I. This complex yielded different kind of structures by switching from excited state to ground state depending on initial structural configuration. Bridged radical always formed I2, whereas classical radical formed parent C2H4I2 molecule. I2 never formed in S1 state. In order to formation of I2, both excitation and transition from exited state to ground state are necessary.

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

Asymmetric Transport Dynamics of Hydronium and Hydroxide: Hydroxide Goes Brownian While Hydronium Hops

Nizam Uddin 최철호[1,*]

경북대학교 일반대학원 화학과 [1]경북대학교 화학과

It has long been conceived that the hydronium (H3O+) and hydroxide (OH-) in aqueous solution move via proton transfer mechanisms, rooted in the Brønsted?Lowry acid?base definition in which they are the proton donor and acceptor, respectively. Various transport mechanisms have emerged from the proton transfer concept. By employing a combined study of experiments and simulations, however, we find that hydroniums undergo proton transfers efficiently even at low temperature (~160 K), whereas hydroxides hardly undergo proton transfer but exclusively take Brownian motions at room temperature. The asymmetric diffusion of hydronium and hydroxide ions recalls the Arrhenius definition of acid?base that emphasizes their respective roles. Our study indicates that hydronium and hydroxide should have distinctly different transport paths, rates, and action ranges in water, which would tremendously impact the thermodynamics and kinetics of biological and chemical systems such as fuel cells.

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발표종류: 포스터, 발표일시: 수 16:00~19:00

Unfolding Transition of Azide Bound Hemoglobin Probed by Vibrational Absorption of the Ligand

LinHanWei 박성철 임만호*

부산대학교 화학과

Unfolding of azide-bound met hemoglobin (HbN_3) was followed by probing absorption band of the bound azide near 2030 cm^{-1} as temperature of the sample was varied from 10℃ to 84℃. Whereas the antisymmetric stretching mode of azide ion in water solution is centered at 2042 cm^{-1} with a full width at half maximum (fwhm) of 22cm^{-1}, that in HbN_3 shows two bands at 2045 (5%) and 2023 cm^{-1} (95%) with much narrower fwhm's. As temperature of the sample increases, the vibrational bands shift toward the lower frequency and their widths become wider. The binding constant (Kb) for $Hb + N_3^- \leftrightarrow HbN_3$ gradually decreases with temperature. But the band intensity for the free azide ion in the mixture of Hb and N_3 abruptly increases near 82℃, indicating that the protein is unfolding with temperature and the Kb for the unfolded protein is much smaller than the folded one. Assuming that the unfolded Hb does not bind the azide ion, the unfolding curve of HbN_3 with temperature was recovered. The unfolding curve shows the melting temperature (T_m) at 82℃ width transition width of 6℃. Considering that the T_m is 66℃ with transition width of 5℃ in HbCO, the azide-bound ferric Hb is structurally more stable than CO-bound ferrous Hb. Structural implication of the anion-bound Hb will be presented.

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발표종류: 포스터, 발표일시: 수 16:00~19:00

A facile way to synthesize one oriented mesoporous WO3 films

Zheng jin you 강영수*

서강대학교 화학과

The transparent WO_3 films with dominant (002) or (200) crystal facet orientations were fabricated on FTO by facile spin coating method via different solutions. The uniform (002)-oriented Bi-doped WO_3 films were composed of the nanoparticles with the size of < 100 nm by spin coating of gel type Bi-H_2WO_6 precursor solution. In addition, the uniform (200)-oriented WO_3 films were made by spin coating of PVP+H_2WO_6 precursor solution. The as-obtained films were characterized by XRD, SEM, TEM, UV-vis and XPS. Especially, their photoelectrochemical properties were checked and they show good performance.

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발표종류: 포스터, 발표일시: 수 16:00~19:00

Enhanced Performance of Dye-Sensitized Solar Cells byβ-NaYF4: 20% Yb3+, 2% Er3+ Up-converting Nanoparticles

신우진 강영수*

서강대학교 화학과

Up-conversion is a process where low-energy photon is converted into a high-energy photon[1]. Up-conversion phosphor can convert infrared light into visible light. In this work, nano-sized β-NaYF4 doped with ytterbium (Yb) and erbium (Er) was synthesized by reflux system using rare-earth oxide precursors. Up-converting phosphor Yb, Er doped β-NaYF4 is the most promising candidate for dye-sensitized solar cells (DSSCs) currently, due to its outstanding up-conversion efficiencies at emissions around ~550 nm which can be efficiently absorbed by the N-719 dye. It can apply into different parts of the DSSCs and enhance its efficiency by using not only visible light, but also infrared light. Further investigation of their optical properties has to be done, along with new ideas for their application into DSSCs. We expect this concept with up-conversion phosphor can be a possible candidate for DSSCs with enhanced performance.

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Synthesis of Tetragonal LaVO4 by Hydrothermal Method and Application to Downconversion Phosphor of DSSC

엄태영 강영수[*]

서강대학교 화학과

Tetragonal LaVO4 is an important rare-earth activators. Downconversion phosphor can convert UV light to Visible light. In DSSC (dye-sensitized solar cell), its efficiency is improved by downconversion compared with the general DSSC system and dye is more stable as from photooxidize. LaVO4 is fabricated by using hydrothermal method. The adsorption of oleic acid on certain surfaces make nanoparticle as a plate shape which is 40×40×10 nm. Well dispersed nanoparticls was obtained into the organic solvent because of the oleic acid. This property makes easy application to dye-sensitized solar cell through coating method. Properties of nanoparticles have been checked by XRD, TEM and photoluminescence.

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발표분야: 물리화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Comparative Study on the Facet Controlled TiO2 Film

엽소진 강영수*

서강대학교 화학과

The preparation of morphology controlled TiO2 single crystals was done by hydrothermal method using HF as capping reagent. The structure and shape of TiO2 crystals were identified with XRD and FE-SEM. The fabrication of the shape controlled TiO2 crystal films with selective facet exposure of (001), (100) and (101) facets was carried out for the comparative determination of the photocurrent values and the efficiency of water splitting. The specific facet control of TiO2 nanocrystals by exposure of selected facet was done by finger rubbing and secondary growth of the film in the seed layer. The comparative study on the effect of selective control of facet exposure has been done to get the higher photoactivity of the single crystals. The fabricated films with the larger exposure of the surface area of {100}, {001} and {101} facets were solar light irradiated to determine photocurrent and photocatalytic property for water splitting reaction. The fabricated films of TiO2 crystals were studied on the structure and optical properties with FE-SEM, TEM, XRD, EIS, diffuse reflectance UV-vis and XPS

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Photoelectrochemical Performance of Cu-doped α-Fe2O3 Nanocrystal Thin Film

안나현 강명종 강영수*

서강대학교 화학과

The photoelectrochemical performance of α-Fe2O3 nanocrystal thin film is changed due to Cu-doping in α-Fe2O3 nanocrystal. Cu-doped α-Fe2O3 doesn’t changed the shape and morphology a lot but it decreases the crystallinity of α-Fe2O3 nanocrystal. This was investigated by checking XRD. As wt% of Cu ions was increased, the peak intensity of each crystalline axis XRD patterns was decreased. The defect sites in the hematite increase, resulting in increase of the trapping sites of the diffusing electrons as well. As a result, the photocurrent density of the α Fe2O3 was decreased. Also, optical absorption coefficient of Cu-doped α-Fe2O3 was decreased.

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Insights into Architecting the Morphology and Structure of Nanomaterial for Enhancing Photo-Catalytic Activity

van thanh khue 강영수*

서강대학교 화학과

Taking advantages of selective adsorption of each particular crystal facet of semiconductor nanomaterials, the morphology-controlled synthesis of various shapes was done by using surfactants or foreigner chemical species. As the results, by using cetyltrimethylammonium bromide (CTAB) which acts as surfactant, dispersed CdS single crystals were obtained via a hydrothermal condition. Strong interaction between the cationic head groups of CTAB and the {001} planes of CdS hexagonal crystals result in a single-crystalline growth along [100] direction. On the other hand, uniform and single-crystalline α-Fe2O3 polyhedral nanoparticles in hexagonal crystal system named truncated hexagonal bipyramid (THB) were fabricated. Under hydrothermal condition, carboxymethyl cellulose (CMC) and hydrazine molecules play roles such as dispersant and capping agents, respectively, during the crystal growth. The optical and magnetic properties of the hematite particles were investigated as well.

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Fabrication and Characterization of (012) Orientated Hematite Thin Film for Solar Water Splitting

강명종 강영수*

서강대학교 화학과

For enhanced photoelectochemical properties of hematite thin film for solar water splitting, manual assembly of hematite nanoparticle to have one-axis orientated, especially on (012) plane. The orientated hematite thin film electrode showed a promising current density of 0.8 mA/cm2. This current density value is six times enhanced comparing with pristine hematite thin film electrode (random orientated hematite film). This is due to existence of surface hydroxyl group proved by Raman spectroscopy and short Fe-O bond revealed by X-ray photoelectron spectroscopy. This work suggested that new noble method for fabricating one-axis orientated hematite film with high photoelectrochemical efficiency for solar water splitting and hematite photoanode for artificial photosynthesis.

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p-n junction between well-aligned ZnO nanotubes and thin layer of BiOI deposited on the ZnO nanotubes

김도윤 강영수*

서강대학교 화학과

Photocatalytic devices by simulating the photosynthesis of plant can be designed as photoelectrochemical cell (PEC cell), which can split the water into oxygen and hydrogen gases. These gases can be used for clean fuels which can solve the lack problem of fossil fuels. The ZnO is a good photoanode which can be applied in many ways because of its various morphologies. In addition, ZnO nanotubes have high surface area so they can be applied in many ways such as formation of high-efficient junction with other chemical materials. The well-aligned ZnO nanotubes are fabricated on the Si(100) substrate by etching the ZnO nanorods which are formed by hydrothermal growth method. The ZnO nanotubes are characterized by scanning electron microscopy and transmission electron microscopy. And finally, p-n junction between BiOI is formed to enhance the photocatalytic property.

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A Study on the Constitution of Dye-Sensitized Solar Cells with NaTi2O4 Photoanode

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Sodium titanate nanobelts have a function of photoanode in dye-sensitized solar cell based on photoelectrochemical properties. By hydrothermal method at 180 ℃ for 24 h, a concentrated NaOH solution is added to Ti(OBu)4, the Ti precursors to synthesize the sodium titanate nanobelts. The formation mechanism of NaTi2O4 nanobelts in the synthetic process has been studied on the control of condition in pH, reaction time, and concentration of precursors. Their optical property and morphology were measured with Ultraviolet-visible spectroscopy, scanning electron microscope, transmission electron microscope, and X-ray diffraction spectrometer. With the optical and morphological traits of NaTi2O4 nanobelts, it has been used as photoelectrode in DSSC. The fabrication of DSSC photoanode with sodium titanate has been done with doctor blade method.

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Interaction of CF3COOH with surface and subsurface hydrogen on a ZnO(0001 ?) single crystal surface

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경북대학교 화학과

The reaction of trifluoroacetic acid with both surface and subsurface hydrogen atoms on ZnO(0001 ?) has been investigated using a temperature programmed desorption (TPD) technique. On a clean surface, CF3COOH is dissociatively adsorbed forming hydroxyl group and trifluoroacetate on the surface. Upon heating, hydrogen atoms are associatively desorbed as H2 at 425 K. Trifluoroacetate is further decomposed to produce trifluoroacetyl fluoride (CF3CFO), carbon dioxide and carbon monoxide at 583 K. We will compare the interaction of both surface and subsurface hydrogen atoms with trifluoacetate on ZnO(0001 ?).

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Adsorptions and Reaction Mechanisms of SO2 and NO2 on Ice Surface

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경북대학교 일반대학원 화학과 [1]경북대학교 화학과

Theoretical calculations have been carried out regarding the adsorption and reaction mechanism of SO2 on ice surface with the help of DFT/6-311++G(d,p) basis set using our QM/EFP scheme. At first SO2 physically adsorbed on ice surface and then H2SO3 formed by chemical adsorption. It was found that reaction barrier depends on surface heterogeneity as well as ice surface model and the net barrier of H2SO3 can be as low as 0.2 Kcal/mol. Reaction barrier found in this study is 18.8 kcal/mol, which is about 3 kcal/mol lower than previous studies indicating that H2SO3 can be easily formed.

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RESOLFT microscopy using photo-switchable organic fluorophores for efficient super-resolution imaging

박재완 권지웅[1] 김성근[*]

서울대학교 화학부 [1]서울대학교 생물물리 및 화학생물학과

In microscopic imaging of biological systems, the reversible saturable optical fluorescence transition (RESOLFT) technique is a uniquely powerful method with its nanometric spatial resolution using photoswitchable fluorescent proteins. We applied the RESOLFT technique to organic fluorophores, which can be in more versatile use, by precisely controlling the imaging conditions to overcome the typical photobleaching problem. We have demonstrated the feasibility of this application by observing the cytoskeletons in fixed HeLa cells, which readily yielded a sub-100 nm spatial resolution.

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Photoexcitation Dynamics of NO bound Ferrous Iron Complex Probed by Femtosecond Vibrational Spectroscopy

권다예 임만호* 이태곤

부산대학교 화학과

Femtosecond vibrational spectroscopy was used to probe photoexcitation dynamics of NO in $Fe^{II}(D_2O)_5NO$ dissolved in D_2O. The NO-bound ferrous Fe complex was prepared by bubbling NO gas to $Fe^{II}Cl_2$ in D_2O. The stretching mode of NO in the complex was peaked at 1810 cm^{-1} with a full width at half maximum of 36 cm^{-1}, red-shifted from that in the gas phase value of 1876 cm^{-1}. The red-shift indicates that the bound NO in the complex has NO^- character upon binding to the ferrous Fe. The nitrosylated ferrous Fe complex shows two absorptions in the visible spectrum peaked at 450 and 600 nm. These bands likely arise from charge transfer between the ligand and the Fe ion. Dynamics of NO geminate rebinding subsequent to photodeligation as well as that of vibrational and thermal relaxation of the complex were probed and compared with those in NO-bound porphyrin found in hemoglobin and myoglobin.

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Hierarchical crystal growth of $BaWO_4$ dendrites

정혜윤 허영덕*

단국대학교 화학과

Three-dimensional hierarchical superstructures of $BaWO_4$ dendrites were synthesized in the water-hexane bilayer system with assistance of barium-oleate complex. The $BaWO_4$ dendrite has a trunk along with *c*-axis and series of four branches perpendicular to the *c*-axis. The higher order branched structures of $BaWO_4$ dendrites formed by increasing temperature. The presence of oleylamine is a critical factor for the formation of hierarchical superstructures of $BaWO_4$ dendrites.

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Covalently-bonded fluorophores with enhanced photostability

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서울대학교 생물물리 및 화학생물학과 [1]서울대학교 화학부

Fluorescence techniques are widely used in bio-imaging because of their non-invasive nature with molecular specificity. However, the finite lifetime of fluorescent dyes severely limits the observation time for events of interest and can also perturb the kinetics and dynamics in a single molecule study. Here we report an efficient way to enhance the photostability of fluorescent dyes by forming covalently linked heterodimers. The photobleaching lifetime of the heterodimers were significantly increased in various imaging buffers. We investigated the photophysical properties of the heterodimers by fluorescence correlation spectroscopy, which clearly showed that the photobleaching quantum yield decreases drastically when two fluorescent dyes are covalently linked.

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The Property and Application of Graphene Oxide(GO) & GO Derivatives Reduced by Femtosecond Laser

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엘투케이플러스 기업부설연구소 [1]한국표준과학연구원 미래융합기술부 의료융합측정표준센터 [2]한국표준과학연구원(KRISS) 양자연구부 분광그룹

We have studied the fluorescence properties of Graphene Oxide(GO) having the dependence on concentration in aqueous solution using transient spectroscopy by femtosecond laser. In ongoing to study we found the change of properties of Graphen Oxide(GO) after UV wavelength irradiation of femtosecond laser. Previously it was reported about the reduction (rGO) of GO without the need for chemical reduction agent or thermal annealing using the method of photothermal reduction via continuous wave xenon (Xe) lamp exposure. Herein, we measured the optical properties Graphene Oxide (GO) and GO derivatives reduced by ultrashort pulses generated from Orpheus and Pharos combinations. Also, we fabricated micro patterned Graphene Oxide(GO) & GO derivatives via photoreduction and patterned on Graphene Oxide(GO) film by using femtosecond micro-processing machine.

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X^-…HO-Y와 X^-…HN-YZ (X, Y, Z = F, Cl, Br)의 Charge-Transfer State의 특성에 대한 양자화학 계산 연구

문자연 안희선 백경구*

강릉원주대학교 화학과

비-공유 상호작용을 가지는 간단한 시스템인 X^-…H-OY 와 X^-…H-NYZ (X, Y, Z = F, Cl, Br) 음이온들의 분자구조 및 진동수 값을 ab initio 방법들과 DFT 방법들로 계산한 후, 이들 중성 분자(X…H-OY 와 X…H-NYZ)의 바닥 전자상태 및 전하-이동(Charge-Transfer) 들뜬 전자상태의 수직-들뜸-에너지, 분자구조 및 진동수를 IP-EOMCC 및 TD-DFT 방법으로 구하였다. 또한 이들 음이온 및 중성 분자들의 해리 한계들(Dissociation Limits)도 계산하여 가능한 해리 경로들의 에너지 특성과 상호 연관성을 조사하였다. 모든 계산에서 Aug-cc-pVTZ 기저 집합을 사용하였다. 음이온의 구조특성, 중성 분자의 바닥 및 들뜬 전자상태의 특성, 그리고 전하-이동 전자상태와 해리 경로들 사이의 연관성 등이 X, Y, Z 에 따라 어떤 경향성을 나타내는지 연구하였다. 본 연구는 전하-이동 상태에 대한 이해를 넓히는데 도움이 될 것이다.

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Theoretical study on the structural and thermodynamic properties of possible secondary structures for alanine polypeptide

임해리 홍주연 함시현*

숙명여자대학교 화학과

Quantitative prediction of the possible secondary structures is important to understand the function of proteins at the molecular level. Among the many possible secondary structures, the α-sheet has been received a great attention because it was proposed as the possible intermediate conformation to form the β-sheet fibrils in the aggregation process. Including the α-sheet conformation, the eight possible secondary structures (3_{10}-helix, α-helix, P_{II}-helix, π-helix, Anti-parallel β-strand, Fully extended β-strand, Parallel β-strand, and α-strand) for alanine polypeptide in gas phase and aqueous phase were investigated by using quantum mechanics and solvation free energy calculations. Based on computational study on structural and thermodynamic properties, we discussed the relative thermodynamic properties which are the thermodynamic stability, Gibb's free energy, enthalpy, entropy, and solvation free energy for the possible secondary structures in gas phase and aqueous phase.

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Analytic functions for two-dimensional diabatic potential energy surfaces with two dissociation channels

안희선 백경구*

강릉원주대학교 화학과

In order to study the non-adiabatic molecular dynamics involving multi-electronic states by using the quantum wave-packet propagation method, the construction of the diabatic potential energy surfaces (PESs) and the coupling term between them is an indispensable prerequisite. Applicability of the previous analytic functions like LEPS to the diabatic PESs should be reexamined because the functions mainly aim at adiabatic PESs. The charge-transfer states especially demand the reconsiderations. A few analytic functions for two-dimensional (2D) diabatic PESs are devised in this work; their flexibility and reliability are tested with respect to the characteristics of PESs such as the relative energies and geometric parameters of important stationary structures and dissociation limits. The results of quantum wave-packet propagations with our new analytic PESs are compared with the corresponding ones of our earlier works for *FH-Cl* [1] and *H_2NH-Cl* [2] with numerical PESs.

[1] H. An, K. K. Baeck, Submitted. (2014).
[2] Y. C. Park, H. An, H. Choi, Y. S. Lee, K. K. Baeck, Theor. Chem. Acc. 131, 1212 (2012).

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$(H_2O_3)…(H_2O)_n$ (n=1-4) 클러스터의 구조, 에너지, 분광학적 특성에 대한 이론적 연구

송희성 김승준*

한남대학교 화학과

Hydrogen polyoxide 중 한 종류인 H_2O_3 와 H_2O cluster $(H_2O_3)…(H_2O)_n$ (n=1-4)의 상호 작용에 대하여 순 이론적 계산 (ab initio), 밀도 범함수 이론 (DFT)의 양자역학적 방법을 사용하여 분자구조를 예측하고, 결합에너지, 그리고 진동 주파수 (vibrational frequency)를 계산하였다. 분자 구조와 진동 주파수는 B3LYP, CAM-B3LYP, MP2 의 양자역학적 방법들을 CC-pVDZ, CC-pVTZ 의 basis set 수준까지 최적화하였으며, 각각의 분자 구조들은 local minimum 구조임을 확인하였다. H_2O_3 로부터의 결합에너지(ΔE)는 각각의 최적화된 분자 구조에서의 에너지 차로 계산하였다.

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Efficient Monte Carlo Simulation Methods: Protein-DNA Binding Systems

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동아대학교 화학과

The lattice-based Monte Carlo simulation method is one of the most efficient methods for the diffusion-influenced reactions. In this presentation, we show that our adaptive jumping distance methods improve the efficiency of the simulation dramatically by reducing the simulation time without loss of accuracy. Since the enhanced Monte Carlo simulation methods are especially practical for long time dynamics where many interesting universal laws can be found, they will be useful for analysis of many diffusion-influenced reactions. These efficient methods are applied to protein-DNA binding systems especially for comparison of different DNA lengths.

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Structural Investigation of Dicyclohexyldiselenide Self-Assembled Monolayers on Au(111) Studied by Scanning Tunneling Microscopy

정혜림 강훈구 박희건 한진욱 노재근*

한양대학교 화학과

Selenium (Se)-based self-assembled monolayers (SAMs) have drawn much interest in nanoscience and technology due to their superior structural and long-range order properties compared to thiol (S)-based SAMs. However, the fabrication of Se-based SAMs requires a special adjustment of the parameters of the preparation procedure. Generally, it was known that the formation of Se-based SAMs is strongly affected by the preparation conditions such as temperature, concentration of deposition solution, and immersion time. Therefore, experimental conditions for obtaining high-quality Se-based SAMs should be considered with care. We investigated the surface structure of dicyclohexyldiselenide (DCDSe) SAMs by using scanning tunneling microscopy. It was found that the ambient-vapor pressure deposition method is more useful to obtain the high-quality DCDSe SAMs compared to the solution deposition method. Under the optimized condition of DCDSe SAMs formed at 50 ˚C for 12 h, we can obtain the high-resolution STM image of DCDSe SAMs with $(2 \times 2\sqrt{10})R27^\circ$ superstructure.

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Formation and Structure of Selenophene Self-Assembled Monolayers on Au(111)

김영우 강훈구 노시은 한슬기 성태현[1] 주가영 노재근*

한양대학교 화학과 [1]한양대학교 나노융합과학과

The formation and structure of slenophene self-assembled monolayers (SAMs) on Au(111) prepared by vapor or solution deposition methods were investigated by cyclic voltammetry (CV) and scanning tunneling microscopy (STM). STM imaging revealed that the surface structures of selenophene SAMs prepared by vapor deposition method were markedly different from those prepared by solution deposition method. Even though both of selenophene SAMs prepared by vapor and solution method give rise to the formation of two-dimensional SAMs through chemisorption, selenophene SAMs prepared by vapor deposition at high temperature contained well-ordered structure and high packing density unlike those prepared by solution deposition. CV measurements showed that reductive desorption peak for selenophene SAMs was observed at around 900~1000 mV, whereas that for thiophene SAMs was observed at around 850~900 mV. This result means that the Se-Au interaction for selenophene SAMs is stronger than the S-Au interaction for thiophene SAMs. We found that 2-D surface strcutures of selenophene SAMs are strongly influenced by preparation method (vapor or solution), temperature, and immersion times.

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Two-dimensional Growth and Structural Order of 4-Methylbenzenethiol Self-Assembled Monolayers Guided by Displacement of Cyclohexanethiols on Au(111)

성태현 강훈구[1] 주가영[1] 노재근[1,*]

한양대학교 나노융합과학과 [1]한양대학교 화학과

Aromatic thiol self-assembled monolayers (SAMs) on metal surfaces have drawn much attention due to their interesting electrical and optical properties that may be applicable in molecular electronics. On the other hand, two-dimensional ordered SAMs of aromatic thiols are strongly required for improving device performance and obtaining reliable data. It is well-known that the adsorption of 4-methylbenzenethiols (4-MBTs) on Au(111) led to the formation of poorly ordered SAMs. In this study, to control structural order of 4-MBT SAMs, displacement technique based on pre-covered cyclohexanethiol (CHT) SAMs as transient layers were used. Scanning tunneling microscopy observation revealed that well-ordered 4-MBT SAMs with $2\sqrt{3}$ x $\sqrt{3}$R80 ° lattice structure on Au(111) surfaces can be obtained via the displacement of pre-covered CHT SAMs on Au(111) by 4-MBT molecules. It was found that 4-MBT SAMs with long-range ordered domains were formed after displacement for 20 min.

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Excluded volume effects in Forster resonance energy transfer and an experimental method to determine the size of excluded volume

양민오

충북대학교 화학과

Forster theory for the ensemble-averaged population of excited chromophores is generalized to include the excluded volume and orientation correlation in the distribution of energy donor and acceptors. The conventional Forster theory assumes a random distribution of energy acceptors around an excited chromophore. This leads to the well-known formula of a stretched exponential decay of population. However, when the concentration of energy acceptors is high, a major part of excited population decays by neighboring acceptors and the molecular correlations between a donor and adjacent acceptors should be properly considered. The primary molecular correlation is created by excluded volume in a molecular pair arising from finite molecular sizes. Within an independent pair approximation, an analytical expression for the excited population is derived and written in terms of a few simple elementary functions which can be used conveniently in the analyses of experimental data. The population decay exhibits transient non-Forster kinetics of an exponential decay at early times and later the Forster kinetics of a stretched exponential one. An experimental scheme to determine the size of molecular excluded volume is suggested. Effects of correlated molecular orientations are shown to be approximately represented by an effective excluded volume.

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Vibrational Forster resonance energy transfer kinetics in liquid water

양민오

충북대학교 화학과

Using a generalized Forster theory, we analyzed vibrational FRET kinetics of excited OH bonds in liquid water. Excluded volume and orientation correlation are found to have opposite effects on the kinetics of vibrational FRET processes. However, the former is more important and the kinetics of vibrational FRET processes becomes slower due to the excluded volume. We found that the decay of survival probability exhibits a kinetic transition from an exponential form at short times to a stretched exponential form at long times. Due to the high concentration of OH bonds in neat water, a majority of intermolecular energy transfer takes place in the exponential regime rather than in the stretched exponential one as usually assumed. Time scales of intermolecular vibrational FRET in water was calculated to be 210 fs at early times and it becomes twice in about 500 fs while the initial time scale of intra-molecular energy transfer to be 480 fs and becomes twice more quickly in about 250 fs. Quantum yields of IVR, intermolecular FRET, and intra-molecular VET were calculated to be 0.413, 0.420, and 0.167, respectively.

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The effect of conjugation in macrocyclic ring on the photophysical properties of a series of thiaaceneporphyrinoids

성영모 김동호*

연세대학교 화학과

Porphyrinoids have had a great fascination for chemists due to their potential applications in photovoltaic devices, photodynamic therapy, and photosensitizers. In porphyrinoids, π-electron conjugation on the macrocyclic framework plays an important role in lowering the overall energy of the molecules and determining the chemical properties. In this regard, numerous researches on the synthesis of modified porphyrinoids which have different macrocyclic π?conjugation pathway such as thiophenoporphyrins have been conducted, but only few studies have been performed to reveal the effect of macrocyclic π?conjugation on their photophysical properties.In this study, we have investigated the influence of macrocyclic π?conjugation pathway in a series of thiaaceneporphyrinoids on their photophysical properties by various spectroscopic measurements and quantum mechanical calculations. Our results will provide insight into controlling the π?conjugation pathway in macrocyclic ring systems.

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Organic Light-Emitting Field-Effect Transistors Based upon p-type Copper Phthalocyanine and n-type Perylene

김대규 오정도 최종호*

고려대학교 화학과

The neutral cluster beam deposition (NCBD) method has been employed to fabricate and analyze ambipolar, heterojunction-based organic light-emitting field-effect transistors (OLEFETs) with a top-contact, multi-digitated, long-channel geometry. Organic thin films of n-type N,N’-ditridecylperylene-3,4,9,10-tetracarboxylic diimide (P13) and p-type copper phthalocyanine (CuPc) were successively deposited onto the hydroxyl-free polymethyl-methacrylate (PMMA)-coated SiO2 dielectrics using the NCBD method. Atomic force microscopy and X-ray diffraction were used to analyze the morphological and structural properties of the organic active layers. A variety of device parameters such as hole- and electron-carrier mobilities, threshold voltages, and electroluminescence (EL) was derived from the fits of the observed current-voltage (I-V) and current-voltage-light emission (I-V-L) characteristics of OLEFETs. The OLEFETs demonstrated good field-effect characteristics, well-balanced ambipolarity, and substantial EL under ambient conditions. The operating conduction mechanism that accounts for the observed light emission is also discussed.

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Pentacene and Perylene-based Complementary Organic Logic Gates

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We fabricated and characterized complementary organic NAND gates through integration of unipolar p- and n-type organic field-effect transistors (OFETs) produced by the neutral cluster beam deposition (NCBD) method. Two active layers of p-type pentacene and n-type N,N´-dioctyl-3,4,9,10-perylenedicarboximide (PTCDI-C8) were successively deposited on hydroxyl-free polymethylmethacrylate (PMMA) dielectric-modified indium tin oxide (ITO) gate substrates. The p- and n-type transistors showed hole and electron mobilities of 0.247 and 7.23 × $10^{?2}$ cm^2/Vs, respectively, in air without encapsulation. Based on the good balance between component p- and n-type OFETs, the complementary NAND gate exhibited high voltage gain, and large noise margin with little hysteresis. Also the NAND gates revealed correct output on and off states for different input conditions.

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Electronic Perturbation of Internal Bridges in Expanded Porphyrins

임종민 김동호*

연세대학교 화학과

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Comparative Study of Exciton Delocalization in pi-Conjugated Linear and Cyclic Oligothiophenes

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In this work, we have provided a comparative spectroscopic study of pi-conjugated linear and cyclic oligothiophenes, to clarify the role of cyclic molecular geometry on the exciton delocalization of pi conjugated systems. For this purpose, we have performed a detailed investigation of the conformational relaxations in the excited-state of linear and cyclic oligothiopehenes by using femtosecond time-resolved fluorescence up-conversion technique. Especially, time-resolved fluorescence anisotropy decay and fluorescence spectra of linear and cyclic oligothiophenes were measured in subpicosecond and picosecond time scale, respectively, to unveil the change of exciton delocalization with regard to the conformational relaxation dynamics such as exciton self-trapping and dynamic planarization processes. Importantly, we have found that, in spite of the same number of subunits, C10 has longer exciton delocalization length than L10, in the course of conformational relaxation dynamics. The ratio of the 0-1 to 0-0 vibronic peak at early times indicates that this result originates from the more planar structure of C10 by ring strain in contrast with L10. Furthermore, as the ring size increases, the breakdown of cyclic symmetry induces the localization of exciton on the subunits of entire ring, but the ring strain still leads to the degree of exciton delocalization as similar to C10. We believe that our findings presented here are applicable to various pi-conjugated molecular materials and suggest a new method to expand the degree of exciton delocalization by suppressing torsional motion.

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Size-dependent Excited-state Torsional Relaxation and Symmetry Recovery Processes in Conjugated Macrocyclic Oligothiophenes

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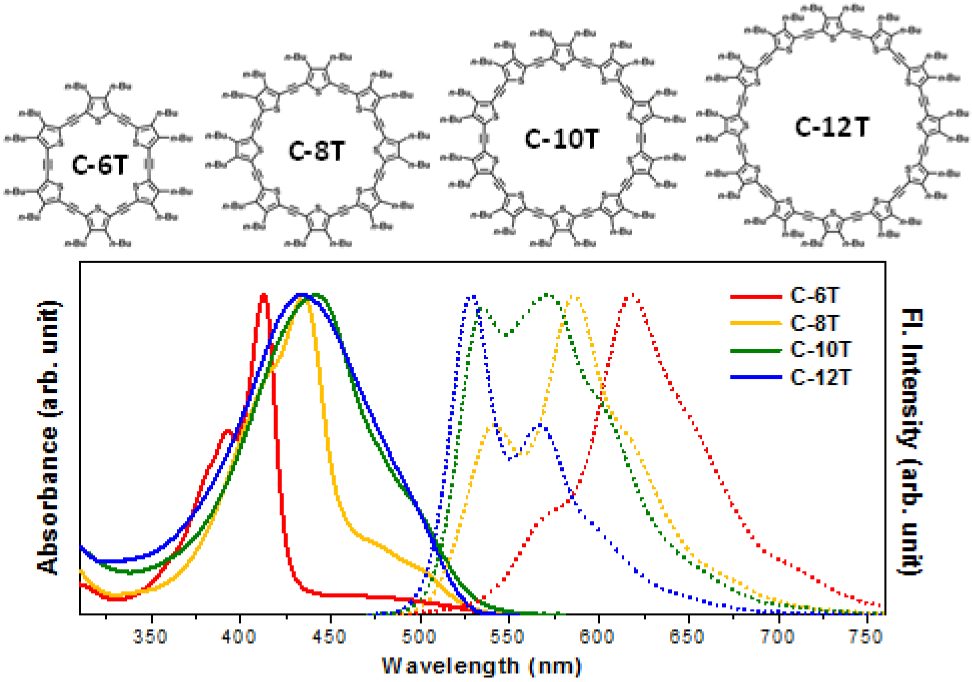
A wide range of researches has been conducted on conjugated oligo-/polymers due to their promising applicability in electroluminescent devices, solar cells, light-emitting diodes, and optical switches. Current academic and industrial scope is limited mostly to linear molecules, yet such systems suffer from their innate shortcomings; structural heterogeneity, defects, size inhomogeneity, all of which downgrade the optoelectric property of the system by breaking π-conjugation pathways. Furthermore, excitonic wavefunction confinement near the center of the molecule, a phenomenon termed “end-effect”, detains full-expression of the designed optical properties in the excited states. In this context, we have prepared a series of cyclic π-conjugated oligothiophenes connected by identical acetylene spacers. These ingenious “end-free” architectures are expected to adopt more planar conformation than their linear counterpart and, therefore, will realize superior exciton delocalization.


C-6T
C-8T
C-10T
C-12T
n-Bu
Absorbance (arb. unit)
Fl. Intensity (arb. unit)
Wavelength (nm)
350
400
450
500
550
600
650
700
750
C-6T
C-8T
C-10T
C-12T

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Gas-Phase Spectroscopy of Laser-Desorbed homo-Tryptophan

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Gas-phase spectroscopy is a way to reveal intrinsic properties of molecules in detail that are otherwise not available, e.g. by spectroscopy in condensed phase. In order to vaporize molecules into the gas phase, the conventional method of choice is heating them up. Though this heating method is very simple in nature, it has a significant draw-back especially for large molecules because large molecules tends to decompose easily by heating. A softer way of vaporization is therefore need, one of which is the laser desorption. We have implemented a laser desorption setup and verified its performance by obtaining the REMPI spectrum of laser-desorbed tryptophan, which is known to fragment easily upon heating. Many amino compounds, including homo-tryptophan, are available only as HCl salts to prevent oxidation. However we show that we can still obtain the spectrum of a neutral amino compound from its salt, by showing that the REMPI spectrum of laser-desorbed tryptophan-HCl is the same as that of neutral tryptophan. Finally we report conformer-specific UV spectra of homo-tryptophan by REMPI and UV-VU hole-burning spectroscopy.

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Influence of Coupling and Charging Energy on Carrier Mobility in Semiconductor Quantum Dot Arrays

최완 심은지*

연세대학교 화학과

We investigated carrier mobility of semiconductor quantum dot (QD) arrays with respect to the properties of QDs and capping ligands. For applications of semiconductor QD, it is important to develop materials with high carrier mobility. As the size of the individual dot becomes larger, the carrier mobility has been known to increase. However, in recent experiments, the carrier mobility of semiconductor nanocrystals have shown non-monotonic trend with respect to QD diameter. In this work, QD arrays are modeled with the size-dependent charging and coupling energy between adjacent dots. Time-evolution of the density matrix is evaluated using the on-the-fly filtered propagator functional path integral method, which is used to extract charge transfer rates which in turn used to evaluate carrier mobility. Conflicting effect of the electronic coupling and the charging energy produces non-monotonic size-dependent trend of carrier mobility. We discuss various factors that define the crossover QD diameter where the carrier mobility reaches its maximum.

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Designed Defects on Two-Dimensional Polymer-Brush by Molecular Frustration

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연세대학교 화학과

Self-assembled two-dimensional molecular architecture contains inevitable defects from molecular frustration. The defects usually deteriorate the functionality, however, by intentionally introducing designed defects employing specific molecular systems, one can generate various kinds of functional structures. For instance, T-shaped rod-coil molecules can be altered to form secondary structures such as hollow tubules or scrolls due to the balance among competitive and conflicting types of interactions. We performed coarse-grained molecular dynamics simulations to quantify the degree of frustration in two-dimensional polymer brush surfaces. In the course of self-organization process, the degree of frustration is low when one type of molecular interaction becomes dominant, whereas the degree of frustration can be made high by introducing a moderate level of conflict in intermolecular interactions. The frustrated two-dimensional surface finally transforms into curved hollow or filled secondary structures to counteract the frustration-driven sheet anisotropy.

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Curvature Controlled Tubule Fabrication Using Grafting-Density Defects

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The nanotube has taken considerable interests as one of potential and cutting-edge materials since it has diverse functionalities depending on the structural properties and characteristics of constituents. We propose a novel method to form and manipulate tubular structures by designing nanosheets that self-roll to designed structures. The nanosheets can be produced by polymer-brush techniques where flexible coils are grafted on flexible lipophobic sheets. When polymer brushes are formed, density and graft defects are inevitable and cause various unwanted outcomes. In this work, we in turn utilize such defects in our favor to self-roll to wanted tubules. As grafting-density defect increases, the size of internal cavity monotonically decreases; however, the rolling-direction becomes irregular when grafting-density defect exceeds 40%. We also found that the direction of rolling can also be controlled by aligning grafting points like a pattern and model nanosheets always roll up in the direction perpendicular to the pattern.

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Bicarbonate Permeability through Ion Channels

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Bicarbonate anion (HCO_3^-) takes the role of major buffer systems in our body by maintaining the pH at 7.4. Epithelial HCO_3^- secretion also hydrolyzes the mucus which protects body from noxious infections. It has been widely known that such infections are closely related to HCO_3^- permeability through membrane and, thus, increasing the HCO_3^- permeability is essential. To evaluate the HCO_3^- permeability through ion channels, the free energy changes relevant to ion pumping are calculated with the Integral Equation Formalism-PCM (IEF-PCM) theory. Molecular structures of various anions including HCO_3^- were optimized with the density functional theory at the level of B3LYP/6-311++G(d,p) in gas and solution phase. In addition, the anion permeability is significantly influenced by the relative size of the anion and pore. We introduce a shifted volume factor model that describes the pore size effect when the charged solutes transfer through ion channels. We found excellent agreement between experimental and calculated permeability when our novel model of the size effect was taken into account to.

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Elucidation of the Structure and Antibacterial Mechanisms for Antimicrobial peptide, LPcin analogs with Enhanced Activities

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한국외국어대학교 화학과

Lactophoricin (LPcin), a cationic amphipathic peptide consists of 23-mer peptide, corresponds to the carboxy terminal 113?135 region of Component-3 of proteose-peptone PP3. LPcin was designed and modified to enhance antibacterial activity using mutation, sequence shuffling for better amphipathic characteristics to improve interacting with bacterial membranes. Three candidates were selected among 11 LPcin analogs which have better antibacterial activity than LPcin. LPcin-yk1 and Lpcin-yk3 has shorter amino acids at C-terminus, LPcin-yk2 has same number of amino acids but has mutant amino acids for better amphipathic characteristics. In order to understand the correlation between the structure of LPcin analogs and antibacterial mechanism, we studied how the modified conformation of LPcin analogs can affect their antimicrobial activity using several biophysical techniques. We successfully overexpressed in the form of fusion protein in Escherichia coli and purified with biophysical techniques like Ni-NTA affinity chromatography, dialysis, centrifuge, CNBr chemical cleavage, Lyophilization and reversed-phase semi-prep. HPLC. In order to verify the purified peptides, we performed Tris-tricine PAGE and MALDI-TOF MS and CD spectrometry. To elucidate antimicrobial mechanisms and dynamics, we use various 1D and 2D NMR techniques using bicelle samples to make membrane enviroments. In here, we will present not only the optimizing processes for high-yield expression and purification, but also solution and solid-state NMR experiments for investigating anti-bacterial mechanisms. The structural calculations of LPcin analogs using Discovery Studio 3.1 and tilt angle prediction based on SAMPI4 Solid state NMR spectra and PISA Wheel pattern were also on the way.

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Expression, Purification, and Structural Characterization of disease related human transmembrane proteins

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한국외국어대학교 화학과

Human transmembrane proteins (hTMPs) are closely related to major disease and the target of modern medicinal drugs. In order to study the structure and function of these hTMPs, it is important to prepare reasonable amounts of proteins. However their preparation is seriously difficult and time-consuming due to insufficient yields and low solubility of hTMPs. We tried to produce large amounts of human amyloid-β (hA?? that is related to the dementia and human melanocortin-4 receptor (hMC4R) that is related to the obesity. The hA? transmembrane protein shows membrane-bound oligomeric state, and the Ca2+-permeable ion channel formation of non-fibril in the cell membrane. It plays a central role in pathogenesis of dementia and Alzheimer disease. The hMC4R has a critical role in part of energy homeostasis. Heterozygous mutations in second transmembrane domain of hMC4R relate in genetic cause of severe human obesity. We succeed to produce the second trans-membrane domain of the wild-type hMC4R (wt-TM2) and mutant hMC4R (m-TM2). Structural characterizations of these proteins in the membrane-like environments were obtained by solution and solid-state NMR spectroscopy. Biological lipid samples with membrane proteins caused a loss of probe efficiency by high dielectric property due to containing large amounts of lipids, water, and salts in solid-state NMR experiment. For these reasons, a specific solid-state NMR probe with high efficiency is built in our laboratory to study biological samples. We could get 1D, 2D SAMMY and SMAPI spectra using this home-built solid-state NMR probe. The structural simulation of hTMPs in membrane environments and Tilt angle calculation based on PISA-wheel pattern of SAMPI4 solid-state NMR spectra are on the way.

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A shortcut binding process in the reaction of 10-23 deoxyribozyme and its effect on the enzymatic turnover rate

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서울대학교 생물물리 및 화학생물학 [1]서울대학교 화학부

10-23 deoxyribozyme is a single-stranded DNA that functions like an enzyme by binding to an RNA target via Watson-Crick base pairing and cleaving a specific RNA sequence. Our previous TIRF studies revealed four distinctly identifiable reaction steps and also found a separate process akin but not identical to a “ping-pong mechanism” that we named a “shortcut binding (SB)” process. The SB process can occur when one end of the cleaved substrate is dissociated while the other end remains bound to the enzyme. Before the dissociation of this remaining part of the substrate, a new substrate can approach the enzyme and bind to its free arm to start its own reaction, making its apparent turnover rate faster. We measured the frequency of the SB process as we varied the substrate concentration to examine the relationship between them that may affect the enzymatic turnover rate.

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Investigation of binding interactions of phenolic compounds with bovine and human serum albumins using fluorescence techniques

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인천대학교 화학과

The interaction of several selected phenolic compounds, gallic and ellagic acids, and propyl gallate with bovine and human serum albumins has been studied using fluorescence spectroscopic methods. Gallic and ellagic acids show a variety of biological activities including antioxidant, anti-inflammatory, and anti-fibrosis, which are in part due to interactions with biomolecules such as proteins or DNA. Propyl gallate is a phenolic antioxidant used in food, cosmetics, and pharmaceutical industries. The interaction of these phenolic compounds with serum albumins was characterized by examining the quenching of intrinsic tryptophan fluorescence of proteins. In addition, the fluorescence spectra of serum albumins exhibit the red shift when the concentration of propyl gallate increases, which suggests complicated interactions including unfolding of the protein. The binding constants and the number of binding sites were determined using the modified Stern-Volmer equation as well as the Scatchard-type analysis, and the nature of binding interactions was discussed. Site marker displacement experiments were also conducted to reveal the binding sites of serum albumins.

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Reconstructing the molecular structures probed by single-molecule defocused wide-field imaging

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연세대학교 화학과

By using optical microscope, single-molecule defocused wide-field imaging techniques and vector calculations, we have unraveled the molecular structural parameters, especially the orientations of emitting dipole moments, angle differences between chromophores and consequently, molecular structures of a series of acetylene-linked perylene bisimide (PBI) macrocycles with different ring size composed of three to six dyes. Furthermore, our findings shown here give that the structural heterogeneities and distortions of cyclic PBI arrays clearly dependent on the ring size. We think that the first direct observations of the molecular structures and flexibilities of PBI macrocycles provide the new way to understand to structure-property relationship for further applications.

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Synthesis of WO_3@TiO_2(Core@Shell) Nano-Structured Materials

정지훈 **Zheng jin you** 강영수*

서강대학교 화학과

Because WO_3 photoanodes absorb a visible light with the stability on photocorrosion, WO_3 have been used for electrochemical water splitting as a photocatalyst by the illumination of solar light. Combining WO_3 with TiO_2 can improve the efficiency for photocatalytic water splitting reaction. Although WO_3 hold a high resistance against photocorrosion, it is not stable at neutral solution. So, a stable layer like TiO_2 should be covered on the surface of WO_3 crystals by forming core-shell structure. By using WO_3 hydrate powder (WO_3H_2O) and Ti source like $Ti(OBu)_4$, we tried to make a crystal type WO_3-core/TiO_2-shell structure by hydrothermal reaction.

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Excited State Proton Transfer of 8-Hydroxypyrene-1,3,6-trisulfonate

허우석

포항공과대학교 화학과

Proton transfer is one of the most important elementary reactions found ubiquitously in chemistry and biology; from acid-base reactions to proton pump at cell-membrane. Of particular interest is to track molecular motions associated with the proton transfer, although obtaining direct information on the proton movement is challenging due to the lack of detection limit in temporal domain. Excited state intermolecular proton trasfer (ESPT) has been an effective experimental approach to study of the proton release of photo-acids because the reaction can be coherently initiated by a short pump pulse. We have employed femtosecond time-resolved fluorescence (TRF) utilizing fluorescence up-conversion experiment providing 50 fs time resolution to investigate the intermolecular proton transfer reaction dynamics and potential energy surfaces associated with it. 8-Hydroxypyrene-1,3,6-trisulfonate (HPTS) has a pK_a close to 0 in the excited state, whereas the pK_a in the ground state is 7.[1] Therefore, upon excitation by 400 nm light, HPTS undergoes ESPT reaction. When dissolved in 4 M acetate buffer solution, it shows intermolecular proton transfer rate under 150 fs, the fastest ESPT reported so far.[2] The thermodynamic cycle of HPTS is characterized by the F?rster cycle shown in Figure 1.Figure 2 displays the TRF spectra of HPTS following the photoexcitation at 400 nm over the full spectral range, which covers the acidic HPTS (PA) and basic HPTS (PB) bands at several time delays. The TRF spectra were fitted by two bands of PA (red) and PB (blue). In buffer, the PB band is clearly evident even at time-zero with considerable amplitude, whereas such a characteristic was absent in water. Surprisingly, TRF of PB in buffer shows oscillations, which can be regarded as the coherent vibrational wave packet motions in the excited state of PB. The nuclear wave packet may be created impulsively by the ultrafast intermolecular proton transfer reaction, that is, the proton transfer from HPTS to acetate ion occurs within the periods of certain vibrational modes. The oscillation spectra shown in Figure 3 were obtained by the Fourier transformation. Molecular dynamics simulations (QM/MM) have been performed to show the detailed molecular picture of the proton transfer. Initial contraction of the distance between the donor oxygen and the acceptor oxygen occurs in 30-40 fs, and the proton jumps in10-20 fs ballistically. This theoretical result is entirely consistent with the experimental isotope dependence of the ESPT rates.References1. Tolbert, L. M.; Solntsev, K. M. Acc. Chem. Res. 2002, 35, 19-27.2. Rini, M.; Pines, D.; Magnes, B.-Z.; Pines, E.; Nibbering, E. T. J. J. Chem. Phys. 2004, 121, 9593-9610.

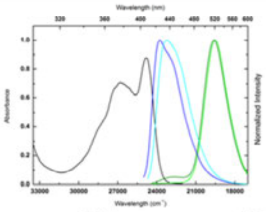

Figure 1. Schematic of the intermolecular proton transfer of HPTS.

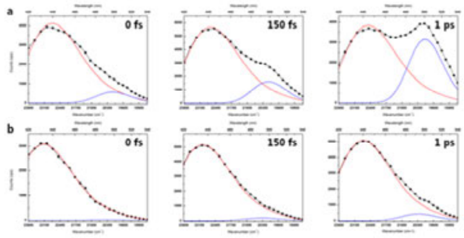

Figure 2. Time evolution of HPTS in (a) buffer and (b) water fitted by PA (red) and PB (blue) bands.

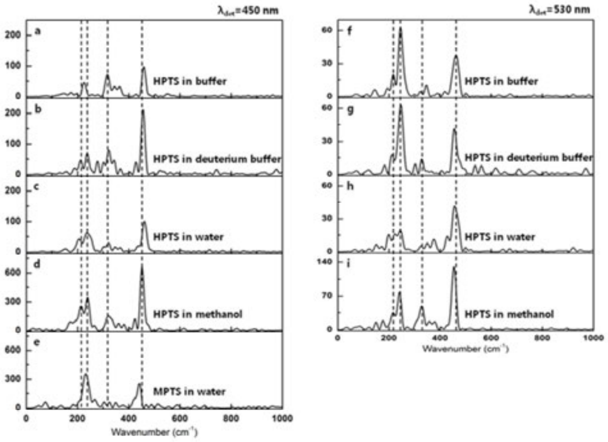

Figure 3. Fourier transforms of the oscillation components in the time-resolved fluorescence of HPTS.

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Mechanistic Insight and Dynamics into the Alcohol Oxidation by Iron-oxo Complex of Non-heme Ligand

Mai Khanh Binh 김용호*

경희대학교 응용화학과

The alcohol oxidation mechanism is calculated by DFT method. Rate constant and KIE for the C-H activation is also calculated with IVTST-M method.

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Photoelectron spectroscopy study on initial stage of photoinduced oxidation of poly(3-hexylthiophene-2,5-diyl) layers on ZnO

정명근 박은지 김영독*

성균관대학교 화학과

The initial stage of the oxidation behaviors of poly(3-hexylthiophene-2,5-diyl) (P3HT) layers on ZnO was studied under visible light irradiation using X-ray photoelectron spectroscopy. . Sulfur of P3HT was partially oxidized into sulfoxide with a sustained ring structure of P3HT in both humid and dry atmospheric conditions. However, the partial oxidation of the P3HT layers resulted in significant changes in optical properties by disturbing inter- and intra-π-conjugation. P3HT underwent more significant change under humid conditions. when the sample was exposed to humid air for extended periods of time, molecular water was incorporated into the P3HT layer. In addition, We obserbed oxidation behaviors with depth from topmost of P3HT layers using angle resolved X-ray photoelectron spectroscopy.

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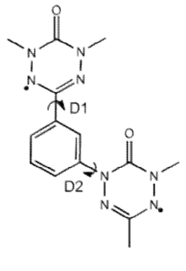
A Density Functional Theory (DFT) Study on Intramolecular Magnetic Coupling in Organic Diradical Systems

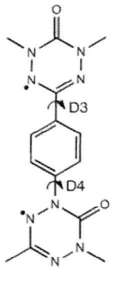
박영근 조대흠 김선경 **SHIHU** 문종훈 **Kang baotao** 이진용*

성균관대학교 화학과

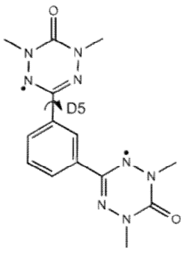
Through the unrestricted density functional theory, the intramolecular magnetic coupling constant (J) values of organic, diradical-based magnet models (S1-S5) were studied. The model systems are based on a series of oxoverdazyl radicals named o-Ver(N) and o-Ver(C), together linked through a benzene coupler. These models are developed on difference of either the connectivity of the radical (C or N) or the geometrical topology (meta- or para-) of benzene coupler. Fair relationship was found between calculated spin density distribution and sign of J value, through which we determined ferro/antiferromagnetic interactions in each system. J values were also observed as dihedral angles between the radical and the coupler were twisted along the molecular plane. We found an overall trend as absolute value of J decreased over increasing torsion angles.



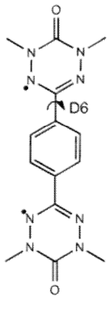
S1
o-Ver(C)-m-benzene-o-Ver(N)



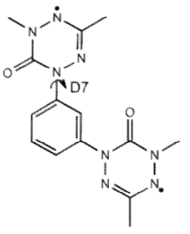
S2
o-Ver(C)-p-benzene-o-Ver(N)



S3
o-Ver(C)-m-benzene-o-Ver(C)



S4
o-Ver(C)-p-benzene-o-Ver(C)



S5
o-Ver(N)-m-benzene-o-Ver(N)

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A DFT study on the enhancement of CO_2 absorption in various blended amine solvents

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성균관대학교 화학과

Carbon dioxide is one of the greenhouse gases that cause the global warming. During last few decades, there were many studies on the amine based solvents for CO_2 removal from the exhaust fumes. Nowadays, the interest in the solvents of blended amines is increased in order to find best blending combination for the CO_2 solubility and regeneration performance. In spite of many studies about the effect of blended amine solvent, there have been no appropriate literature data for understanding about the reaction mechanism and the reason of performance enhancement. In this study, the DFT calculation (B3LYP / 6-31G*) was conducted about the mechanism of carbamic acid formation from CO_2 absorption process in various amine-based solvents. The reactants were CO_2 and amines (MEA, DEA, PZ, AMP, AEEA and DETA) and the reactions were designated without or with catalyst (water or amine). These catalysts play a role as proton donor and accepter, namely, they transfer proton form amino group of amine to oxygen of CO_2 moiety. Amine catalyzed carbamic acid formation in reaction of CO_2 and MEA in various amine-based solvents is preferred compared with water catalyzed and non-catalyzed process that many studies have focused. Moreover, amine catalyzed process can be applied to understand the enhancement effect of CO_2 absorption in blended amine solvents. The enhancement effect on the CO_2 absorption by additive amines was in the order of PZ > AEEA > DETA > DEA > AMP based on the activation energy, which is in excellent agreement with experiment. Our work should be useful in choosing a proper blended amine solvent for better CO_2 absorption.

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C60 Fullerene을 수소 저장체로 사용 했을 때의 물리화학적인 성질

김성후* 이기학[1]

원광대학교 자연과학대학/바이오나노화학부 [1]원광대학교 화학과

Fullerene 은 수소 저장체로 사용 될 수 있는 잠재적 물질이다. fullerene 속의 수소는 다양한 이성체구조를 형성 할 수 있다.Fullerene cage 속에 존재 할 수 있는 수소 분자들의 분자간 상호작용 이성체 구조를 연구하였고, 수소를 저장 했을 때의 fullerene 과의 어떤 상호작용이 나타나는 가에 대한 여러 물리화학적인 특성들 양자화학적 방법으로 연구 하였다.

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Single Chirality Separation of Single-Walled Carbon Nanotube Using Flavin Mononucleotide by Density Gradient Ultracentrifugation

장명수 주상용*

연세대학교 화학과

As-synthesized single-walled carbon nanotubes (SWNTs) are typically highly agglomerated and heterogeneous in physical properties, thereby individual dispersion and subsequent separation of SWNTs with single chirality and identical properties are critical steps enabling various high-end applications such as electronic devices and biological applications. We utilize flavin mononucleotide (FMN), derivative of riboflavin (vitamin B2), to separate a single chirality of SWNTs. When FMN wraps SWNTs in helical pattern, π-π interaction and hydrogen bonding between FMN moieties and graphene sheet of carbon nanotube sidewall allows tight binding . The separated single chirality SWNT from FMN-suspended SWNTs were enabled by density gradient ultracentrifugation (DGU) method, according to both sedimentation coefficients and buoyant density, related to binding affinity between FMN surfactant and various chirality of SWNTs. Unlike other surfactant system as sodium cholate (SC) DGU showing diameter-dependent sorting tendency, FMN DGU system displays sorting tendency according to binding affinity to SWNTs (i.e., SWNT chirality with higher FMN binding affinity located in lower depth). Since separation mechanisms of SWNTs by DGU are not fully understood yet, we expect to reveal the DGU mechanisms by new surfactant system. Separation of various single chirality SWNTs with high purity is undergoing.

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Molecular Dynamics Study on the Zn Ion Induced Conformation Changes of Amyloid β-peptide and E22Δ Mutation

SHIHU Kang baotao 문종훈 박영근 김선경 조대흠 이진용*

성균관대학교 화학과

The aggregation of amyloid β-peptide (Aβ) has been associated with the pathogenesis of Alzheimer's disease (AD). Although pristine amyloids seem to be the main neurotoxic substances, more and more evidences have indicated that metal ions, especially Fe, Cu, and Zn, play an important role in AD pathogenesis. Meanwhile, some studies have proposed that the interaction between metal ions and Aβ peptides could facilitate their aggregation. The effects of Zn ion on the structural properties of Aβ peptide have been intensively studies. Nevertheless, it still remains unclear that how it affects the structural properties to induce aggregation. In this work, molecular dynamic simulations were implemented to elucidate the changes of structural properties as the result of Zn ion coordination. Here, wild type Aβ42 and their E22Δ mutation were taken into account. To achieve our goals, all the calculations were carried out by Amber 12, except the force field applied in the active center (Zn coordinated residues, parameters were obtained by M06/6-31+G* level using a suite of Gaussian 09 program). Our results show that Zn coordination can stabilize both the Aβ42 and E22Δ mutation. Compared with wild type Aβ42, E22Δ mutation make structural properties became more feasible to aggregate owing to the sheet formation. Moreover, in mutation models, Zn coordination can decrease helix formation and increase turn structure, which could benefit to produce the oligomers and aggregation. The structural properties of E22Δ mutations with Zn ion reported here may provide useful information to understand the influence of Zn ions on Aβ peptides aggregation, and it's useful for the development of new drugs to cure Alzheimer's disease.

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Characterizing the Structural and Thermodynamics Properties of Aβ40 and Aβ42: Molecular Dynamics Simulations and Solvation Thermodynamics Analyses

임슬기 함시현*

숙명여자대학교 화학과

Physiological 40-residue and 42-residue amyloid-beta peptides (Aβ40 and Aβ42) are major components of amyloid plaques associated with Alzheimer's disease. Although they differ in only two amino acid residues at the C-terminal end, Aβ42 is much more prone to aggregate and more toxic than Aβ40. To investigate the molecular origin on the differences in the aggregation propensities between those two peptides, we perform the fully atomistic, explicit-water molecular dynamics simulations as well as the integral-equation theory of liquids for solvation thermodynamic analysis. The results indicate that Aβ42 displays higher β-sheet contents and is more rigid in C-terminal region compared to Aβ40. Based on the solvation free energy analysis, Aβ42 is more hydrophobic than Aβ40. This is attributed to the dehydration of the backbone caused by the formation of β-sheet structure at the C-terminal region. Our finding can rationalize why Aβ42 is more prone to undergo self-assembly than Aβ40.

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Single Nanoparticle-Attached Tips for Tip-Enhanced Raman Spectroscopy

김웅 김지환[1] 박준원[*]

포항공과대학교 화학과 [1]서울대학교 화학과

Structural characterization of biochemical samples on the nanometer scale is becoming more important in life science and nanotechnology. Advantages of tip enhanced Raman scattering (TERS) include no necessity of labeling, non-invasive nature, high specificity, and ultra-sensitivity. Throughcombining Raman spectrometer, confocal microscope, and atomic force microscope, limited sensitivity of conventional Raman spectroscopy can be overcome. In this TERS setup, an appropriately prepared metallized (silver, gold) AFM tip plays a key role. The crucial part of the TERS experiment is how to make the best probe maximizing the efficiency. Several approaches have been reported to produce TERS probes, but the best one is yet to come. We reported that a dendron-modified AFM tip guarantees truly single molecular interaction during the force measurement. In particular, the approach demonstrated that picking a single stranded DNA was accessible, and a gold nanoparticle tethered at the DNA was visualized with transmission electron microscope.1,2Because it is necessary to have a single nanoparticle of an appropriate size to enhance TERS signal sufficiently, various silver staining conditions were examined to convert the picked gold nanoparticle (ca. 5 nm) to a particle of 60 nm diameter.As a preliminary study, thus-prepared TERS tip (with a particle of gold-silver core-shell structure) generated a stronger signal than the tip prepared through e-beam coating. After optimizing the structure, size, and crystallinity of the particle on the AFM tip of TERS, the probe will be applied for the graphene based nanoelectronic device and nano-material field.

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Exchange Symmetry, Fluctuation-Compressibility Relation, and Thermodynamic Potential X of Quantum Liquids

임유림 박성준 김지현 성재영*

중앙대학교 화학과

Liquid helium does not obey the Gibbs fluctuation-compressibility relation, which was noted more than six decades ago. However, still missing has been a clear explanation about the reason of the deviation or the correct fluctuation-compressibility relation of the quantum liquid. Here, we present the fluctuation-compressibility relation valid for any grand canonical system. Our result shows the deviation from the Gibbs formula arises from a non-extensive part of thermodynamic potentials. The particle-exchange symmetry of many-body wave function of a strongly degenerate quantum gas is related to the thermodynamic extensivity of the system; a Bose gas does not always obey the Gibbs formula while a Fermi gas does. Our new fluctuation-compressibility relation works for classical systems as well as quantum systems. This work demonstrates the application range of Gibbs-Boltzmann's statistical thermodynamics can be extended to encompass non-extensive open systems without introducing any postulate other than the principle of equal a priori probability.

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Effect of product decay rate on product number fluctuation in Nonrenewal birth process

양길석 김지현 성재영*

중앙대학교 화학과

We study how the decay rate of product modulates the product number fluctuation in nonrenewal birth process. Based on a generalized master equation where creation rate fluctuations encompass a whole range of disorder from dynamic to static limit, we can exactly calculate the moments characterizing the counting statistics of product entities. Correctness of the analytic results is confirmed by stochastic simulation results. Our analyses show that the dynamic non-Poissonian indicator for the product number fluctuation undergoes a kinetic phase transition around the relaxation time of not a creation rate but the associated hidden variable from fully heterogeneous regime to renewal-like regime. The latter regime shares the characteristics of renewal kinetics that is a constant Mandel's Q Parameter over time. It is clearly shown that faster the hidden variable relaxes to its steady state or slower the product decay, more extended the renewal-like kinetic phase is, while in the opposite limit, the renewal-like phase no longer exists. It is also shown that the product decay rate can amplify or depress the product number fluctuation in the renewal-like regime in comparison with the randomness of reaction time interval distribution.

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Crossover from Super-Poissonian to Sub-Poissonian Counting Statistics of Non-renewal Reaction Events

송상근 양길석 김지현* 성재영*

중앙대학교 화학과

We present a theory of consecutive vibrant reactions that l-time intermediate reactions produce one product molecule and each reaction event is coupled to dynamically fluctuating environmental states. The latter is an essential ingredient required to precisely delineate the very heterogeneous reaction systems like living cells. For these genuinely non-renewal reaction event processes, general expressions of time interval distribution between two consecutive product creation events and time-dependent moments of product number are obtained. When environmental processes occur in a confined space, their practical expressions can be also obtained in the matrix representation with help of eigenfunction expansion. For model systems, theoretical predictions and stochastic simulation results are shown to be in excellent agreement with each other. Here, for a given static Fano factor of reaction rate, the inverse relaxation time λ of environmental process and the number l of intermediate steps per product creation control statistical properties of product creation time intervals and product number fluctuations, which are respectively characterized by randomness R and Mandel's Q parameter. For both parameters, their steady-state values decrease with λ or l. As λ increases, a crossover from super-Poissonian to sub-Poissonian statistics of product number fluctuations occur at smaller l. Interestingly, even though the time interval statistics follows sub-Poisson for l >1, there exists the regime bounded by $Q = 0$ in (λ,l) space, where the number statistics follows super-Poisson. This is a special characteristics of non-renewal reaction event processes beyond the scope of renewal processes.

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Monte Carlo Study on the Drying Transition between Two Hydrophobic Surfaces

장지혜 김효정 장준경[1,*]

부산대학교 나노융합기술학과 [1]부산대학교 나노소재공학과

The drying of hydrophobic cavities is believed to play an important role in many natural phenomena, such as protein folding, the opening and closing of ligand-gated ion channels, and adhesion and colloid stability. However, simulations of drying transition have been limited to smooth, flat surfaces, although most surfaces are rough. In this study, we investigated the drying of confined water between hydrophobic surfaces by using a lattice gas Monte Carlo simulation. Considering two different types of surface geometry (plate-plate and hemisphere-plate), we studied an attractive force behavior and a critical distance for cavitation. We also introduced an atomic scale (smaller than 1nm) roughness on the surfaces.We found that in both case geometry with small roughness shows a stronger attractive force behavior and a longer critical distance than other geometry. This result suggests that the rough surface enhanced hydrophobicity.

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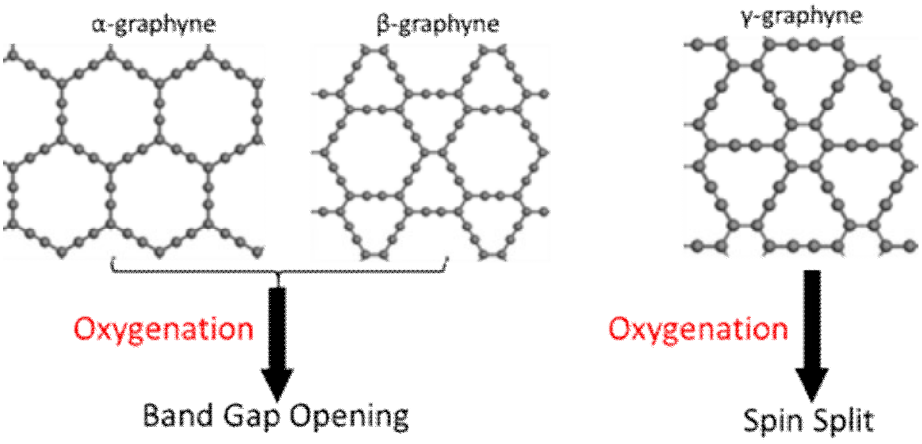
Oxygen Adsorption on Single Layer Graphyne by DFT Study

Kang baotao 문종훈 김선경 박영근 조대흠 SHIHU 이진용*

성균관대학교 화학과

Graphyne is a rising two-dimensional (2D) carbon allotrope with excellent electronic properties. In this paper, theoretical calculations were performed to study the corresponding electronic properties of the oxygenated graphyne. Atomic oxygen when binds to the carbon atom of graphyne forms a stable oxide, with a much larger binding energy compared to that on graphene. Owing to the oxygen adsorption, the α- and β-graphyne change from a zero-band-gap material to a semiconductor as indicated in the band structure calculations. Moreover, spin split was observed from the band structure of the oxygenated γ-graphyne. These electronic properties are tunable by altering the oxygen coverage through changing the supercell size. Our results based on the first-principles calculations imply that oxygenation is a promising method to functionalize graphyne to achieve designated properties.



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Molecular Dynamics Study on the Wetting Properties of Hydrophobic Pillar Surface

ZHANGZHENGQING 김효정 장준경[1,*]

부산대학교 나노융합기술학과 [1]부산대학교 나노소재공학과

Using molecular dynamics simulation, we studied the wetting properties of a surface textured with hydrophobic nanoscale pillars, in order to mimic super-hydrophobic surface properties such as luffas, water strider legs and lotus leaves. The drying transition of water confined between square or circular pillars was related to the Wenzel (WZ) to Cassie-Baxter (CB) transition of a water droplet deposited on periodic pillars. The inter-pillar spacing at which the drying occurs was compared to that predicted from the continuum theory. Such a comparison revealed that the line tension plays an important role in the drying behavior of the present nm-sized pillars. The water molecules near the pillar walls were layered and ordered in orientation. In the CB-to-WZ transition, the surface of water slowly penetrated into the inter-pillar gap until it reached the half height of pillar, and the rest of the transition was relatively quick.

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Wetting Behavior of Regularly Structured Nanoporous Gold Surfaces

<u>Matin Mohammad Abdul</u> 김효정 **ZHANGZHENGQING** 장지혜 장준경[1,*]

부산대학교 나노융합기술학과 [1]부산대학교 나노소재공학과

In this study we report a systematic molecular dynamics study results on the relationship between surface structure and wetting state of regularly ordered nanoporous gold surface. The wettability of the porous gold surface is significantly changed from hydrophilicity to hydrophobicity by increasing the thickness ratio. We find that, as the thickness of the porous gold surface increases up to the radius of the pores, the apparent contact angle for coarse grained water on the surface increases from 73° on the flat gold surface to more than 110°, and then with increasing thickness above the radius of the pores the apparent contact angle decreases back toward 73°.We show that these changes in the apparent contact angle agree with the model of Cassie and Baxter for nonwetted surfaces even though the gold surface itself is hydrophilic. The results are described in the context of both the Wenzel and Cassie models for wetting rough surfaces. We also show that the apparent contact angle is independent of the diameter of the pores over the range of 4 to 8 nm. This study clearly shows the change of a hydrophilic surface (θ90°) purely control of the surface topography. This study could provide further insight into the wetting mechanism of roughness-induced wettability and practical guides for the design of variable macroporous surfaces with controllable wettability.

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Wetting behavior of water confined between hydrophobic pillars

김효정 장준경[1,*]

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The wetting properties of water confined between hydrophobic pillars was studied by using the lattice gas Monte Carlo simulation. The wetting behavior of water is related to the Cassie-Baxter (CB) to Wenzel (WZ) transition of a droplet on a rough surface. We simulated a periodic array of dome pillars, in order to mimic the surface of lotus leaf. The inter-pillar spacing that gives wetting shows a turnover behavior with increasing the width of pillar, in agreement with the continuum theory. We found that the inter-pillar gap is sometimes partially filled with water. This is similar to the metastable droplet partially penetrating into the inter-pillar gap previously reported.

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A single-molecule study of optical and dynamic properties of myoglobin in trehalose-water matrixes

설수현 송승민 조한국 정병서*

인천대학교 화학과

In this study, the single molecule detection technique is used to investigate the optical and dynamic properties of myoglobin complexed with a fluorophore, carboxytetramethylrhodamine (TAMRA) or rhodamine B (RhB), in trehalose-water matrixes. Trehalose, a nonreducing disaccharide of glucose, provides an interesting medium for biological applications due to its ability to stabilize proteins. The fluorescence properties of myoglobin-TAMRA and myoglobin-RhB conjugates are expected to provide information on dynamic behaviors of myoglobin and the heterogeneity in trehalose films. Fluorescence images of single myoglobin conjugate molecules were recorded as a function of time, and the fluorescence emission characteristics, in particular, the fluorescence-intensity histogram and bleaching pattern were analyzed. Also, efforts were made to discern the differences in the fluorescence characteristics depending on the drying condition of trehalose films. These results were compared with those observed from single TAMRA and RhB molecules in trehalose.

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Femtosecond transient absorption spectroscopy with the white-light continuum probe

강동구 정다희 김상규*

한국과학기술원(KAIST) 화학과

The experimental set-up for the time-resolved transient absorption measurement has been constructed using pump-probe spectroscopy technique with femtosecond pulses at the repetition rate of 1 kHz. Due to the reappearance experiment we have carried out measurement on the free base tetraphenylporphyrin (H_2TPP) in the benzene solution by pumping the Soret band. The position of zero time and the instrument response functions of 200 fs was confirmed by using optical Kerr shutter technique resulted from birefringence effect of CS_2 and D_2O. Probe beam in the broad spectral range is used to observe the time-resolved absorption spectra of the each fixed time by using white-light continuum generation through 3 mm CaF_2 or sapphire plate. The ongoing progress is going to investigate the ultrafast excited-state dynamics by optical density of transient absorption spectra of the target molecules such as nanoparticles and biomolecules following excitation at 266 nm and probing in the UV/Vis region (350-650 nm) at various pump-probe delays.

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Exploration of new photoisomerizing dyes for the detection of early-stage insulin oligomers

이휘인 이민영*

이화여자대학교 화학나노과학과

Insulin monomers associate progressively to form oligomers and fibrils which are known to be a primary cause of Type 2 diabetes. Detection of insulin aggregates by any means has been an important issue for the diagnostic purpose. Here we have prepared insulin amyloid oligomers using a well-defined protocol and their sizes were characterized by high resolution AFM as a function of incubation time. By using a time-resolved fluorescence technique, we explored DASPI series, photoisomerizing fluorescence dyes, as new probes to monitor the early stage of insulin amyloid oligomers. We have observed that the fluorescence lifetime of DASPI dyes exhibited a significant increase as bound to amyloid oligomers in comparison with the monomeric state in buffer. On the basis of the molecular structure of oligomer aggregates, we described the binding mode and association constant of the DASPIs to aggregates, which may provide an important step to access molecular interactions between small molecules and insulin oligomers.

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Electronic Spectra of 3-cyanoindole-(H2O)n (n=0-5) Studied by IR-dip Spectroscopy in the Gas Phase and Computational Calculations

민아름 안아름 문철주 이지훈 김성근[1] 최명룡*

경상대학교 화학과 [1]서울대학교 화학부

3-cyanoindole (3-CI) as a derivative of indole has important intrinsic properties for its enormous biological activities in biological systems. In our previous studies, we have identified one 3-CI conformer via the REMPI and UV-UV double resonance spectroscopic studies in the gas phase experiments. In this study, we have further investigated 3-CI-(H2O)n (n=0-5) clusters. For 3-CI-(H2O)1, a clear identification of the two conformers of 3-CI-(H2O)1 was obtained by REMPI and UV-UV hole-burning spectroscopy. Further structural information for 3-CI-(H2O)n (n=0-5) was characterized by IR-dip spectroscopy in the range of 2800-4000 cm-1. We have also calculated the optimized structures of 3-CI-(H2O)n (n=0-5) clusters by density functional theory (DFT). Here reports the structural information of 3-CI-(H2O)n (n=0-5) clusters by comparing the each IR-dip spectra and those from the theory. Further investigation on the intermolecular hydrogen bonding of 3-CI-(H2O)n (n=0-5) clusters will be investigated and discussed by IR-dip spectroscopic studies in this poster.

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The effect of organic additives on the surface of cathode at high voltage condition

신수현 박연주 정영미* 최현철[1]

강원대학교 화학과 [1]전남대학교 화학과

Recently lithium-ion batteries have been attracting attention due to their high energy density and long cycle life. As the applications of lithium-ion battery have developed continuously, safety is one of the major issues. Li-ion battery has stability problem under high voltage condition and it is known that is because of distortion of cathode structure, formation of insulating film, and generation of gas and heat during charge-discharge process. To improve the stability of cathode at high voltage, we investigated the surface-electrolyte interface (SEI) film on the cathode at high voltage using organic additives such as vinylene carbonate (VC) and fluoroethylene carbonate (FEC) in Li-ion battery. In this study, we figured out the effect of additives on SEI film in Li-ion battery by using charge-discharge testing, electrochemical impedance spectroscopy (EIS), cyclic voltammetry and spectroscopies.

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Investigation of the Potocatalytic Dgradation of hexachlorobenzene(HCB) on a Metal oxide Nanoparticles

이슬기 최명룡*

경상대학교 화학과

Metal plates(Ti and Zn) were ablated by a pulsed Nd-YAG laser to produce nano-structured metal oxide compounds in deionized water in the abscence of any surfactants or catalysts. The structural and morphological properties of the metal oxide nanoparticles were characterized by X-ray diffraction(XRD), field-emission scanning electron microscope(FE-SEM), transmittance electron microscope(TEM). The photocatalytic degradation of hexachlorobenzene(HCB) was carried out on metal oxide nanoparticles(NPs) under UV irradiation in solutions. The photocatalytic conditions, including the amount of metal oxide NPs, irradiation time and the intensity of light were optimized. The products of dechlorination reactions and reaction paths were analyzed by gas chromatography(GC).

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Theoretical Studies of 3-Cyanoindole-(H2O)n (n=1-10) Clusters

안아름 최명룡*

경상대학교 화학과

Indole is an aromatic heterocyclic organic compound, consisting of a six-membered benzene ring fused to a five-membered nitrogen-containing pyrrole ring. It is also a popular component of fragrances and precursors in many pharmaceuticals. In this study, theoretical calculations of 3-Cyanoindole (3-CI) and its water clusters with their size up to 10 water molecules are conducted to aid in the spectroscopic analysis in this laboratory. We calculated the 3-CI-(H2O)n (n=1-10) clusters using density functional theory (DFT) with a 6-311++G(d,p) basis set and obtained several low minimum energy structures of each 3-CI-(H2O)n cluster, including global and low-lying energy local minimum isomers. We further carried out the excited state calculations for the corresponding 3-CI-(H2O)n (n=1-10) cluster using time dependent-DFT (TD-DFT). The excited state structures and transition energies of 3-CI-(H2O)n (n=1-10) clusters obtained in this work can be helpful to accommodate the experimental observations. Also Franck-Condon simulation for the S0 → S1 transition of 3-CI monomer is presented for the vibrational analysis. The scaled harmonic frequencies are in good agreement with the experimental values.

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Theoretical study of pyrene-based complexes used as chromophores for organic light-emitting diodes

김동희* 이상희 **Mannix Balanay**

군산대학교 화학과

We have conducted a theoretical assessment of the photophysical properties of a series of pyrene-based complexes with subtituents at the 1,3,5,9- and 1,3,6,8-positions. We have employed density functional theory (DFT) and time-dependent DFT is used to calculate the photophysical properties using different hybrid and long-range exchange-correlation functionals together with the dispersion corrections. The verification of the ground-state geometries was based on the X-ray structures. Among the exchange-correlation functionals, B3LYP-D, a dispersion corrected B3LYP, produced the closet correlation with the X-ray data while optimizing the complexes using LC-wPBE produced the largest deviation. For the absorption energies, the best agreement with the experimental result is with the use of CAM-B3LYP functional followed closely by the wB97X-D functional. Calculating using the standard B3LYP functional produced the worst correlation with experimental absorption energies. This study would eventually pave way to a computational protocol that could design new pyrene complexes for blue organic light-emitting diodes.

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Effect of Protonation on the Molecular Flattening of Cationic Porphyrin TMPyP

문혜윤 심상덕*

순천대학교 화학과

We have studied the interaction between the protonated form of cationic 5,10,15,20?tetrakis(1-methyl-4-pyridinio)porphyrin (TMPyP) and negatively charged reduced graphene oxide (rGO) by UV-Vis and fluorescence spectroscopies. The protonated TMPyP exhibits smaller bathochromic shift of the Soret band than its free base, indicating that the extension of pi-conjugation in protonated species is smaller than that of free base TMPyP. Since the flattening (i.e., the rotation of pyridinium groups toward the coplanar conformation with respect to the porphyrin ring) is mainly responsible for the extension of pi - conjugation, the smaller bathochromic shift in protonated species can be explained by less twist of pyridinium groups from the original position. Meanwhile, fluorescence quenching efficiencies for both protonated and free base species are very similar, implying that the interaction between the porphyrin moiety and the rGO sheet in protonated species is so significant as in free base.

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Micro-phase separation of mixed long chain primary alcohols observed by IR spectroscopy and differential scanning calorimetry

서성욱 조한국* 정병서

인천대학교 화학과

In this paper, we report micro phase separation in the binary solid solution of alcohol observed by IR spectroscopy and differential scanning calorimetry (DSC). The IR spectra of alcohol/alkane solutions clearly show fast phase separation on the basis of the band splitting of the methylene scissoring and rocking bands, regardless of the concentration ratio and difference in chain lengths. The DSC heating curves also reveal at least two strong endotherms unlike the previously studied n-alkane mixtures. Spectral variations indicate that the endotherm observed at the lowest temperature corresponds to the fast phase separation. All these results lead us to believe that long chain alcohol and n-alkane segregate immediately on quenching of the liquid mixture, in contrast to the slow changes in n-alkane solutions. In comparison, alcohol/alcohol solid solutions lead to sluggish segregation and large dependence on the difference in chain lengths. The match in chain lengths cannot overcome the difference in functional group in these alcohol solutions.

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Conformationally resolved structures of jet-cooled phenacetin, and its hydrated clusters

문철주 민아름 안아름 이지훈 김성근[1] 최명룡*

경상대학교 화학과 [1]서울대학교 화학부

Phenacetin (PA) is one of the typical synthetic fever reducers as similar to acetaminophen (AAP), a major ingredient of Tylenol. PA and AAP are both derivatives of acetanilide (AA), substituted by ethoxyl group and hydroxyl group in the para position of AA, respectively. In this work, we present the conformational investigations and photochemistry of jet-cooled PA and its 1:1 hydrates using resonance enhanced multi photon ionization (REMPI), UV-UV hole-burning and IR-dip spectroscopy. Moreover we calculated the optimized structures of PA and its 1:1 hydrates by density functional theory (DFT). Here, we report the structural information of PA and its 1:1 hydrates with an aid of the experimental data and the ab initio calculations.

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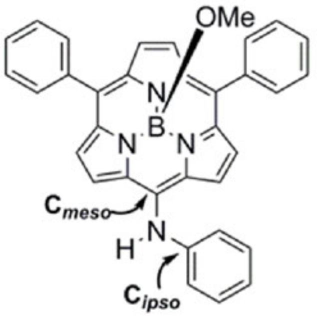
Two Modes of Photoinduced Twisted Intramolecular Charge Transfer in meso-Arylaminated Subporphyrins

차원영 김동호*

연세대학교 화학과

we have investigated the two modes of photoinduced twisted intramolecular charge transfer (TICT) reactions in meso-arylaminated subporphyrins by temperature controlled steady-state and time-resolved absorption/fluorescence experiments along with quantum chemical calculations. While the fluorescence quantum yield of 1 was recorded to be rather high, subporphyrins 2 and 3 were non-fluorescent regardless of degree of solvent polarity. Interestingly, as the temperature decreases from 297 to 107 K, 2 and 3 revealed remarkable fluorescence recovery, which suggests the restricted rotational freedom in the excited-state prevents the charge transfer processes with maintenance of the locally excited-state population. Moreover, calculations of energy minimized structures of the S1-states strongly suggest TICT phenomena in their excited-state dynamics. In femtosecond transient absorption experiments, 1 revealed the slow TA decay in accord with its long fluorescence lifetime and high fluorescence quantum yield. In contrast, 2 and 3 showed the fast TA decay dynamics with significant spectral changes, which have been interpreted in terms of initial formation of locally excited states and their transformation into TICT states.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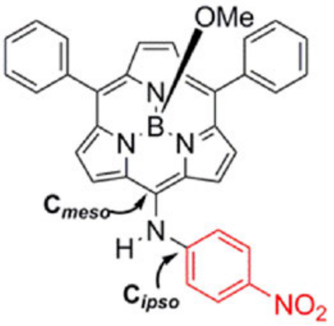
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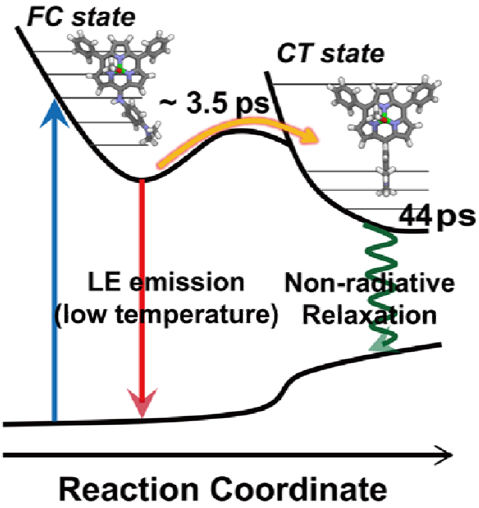
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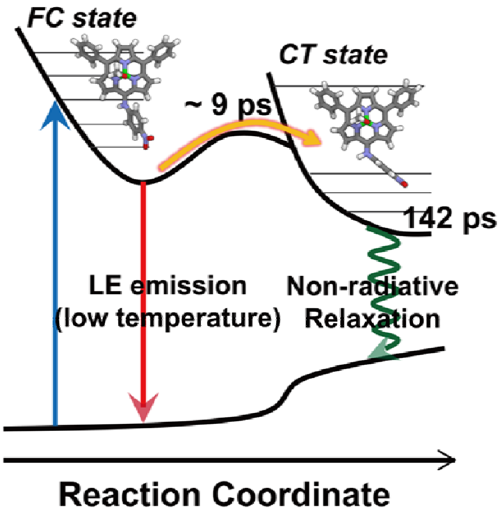
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Synthesis of different shapes of the gold nanoparticles by using drug molecule Isoniazid (INH) and its catalytic and SERS applications

KunwarVikram 정영미*

강원대학교 화학과

Gold nanostructures have been attracting from the several years, due to their fascinating optical, electrical, and chemical properties. These properties are highly dependent on morphologies, such as shape and size, consequently a large number of gold nanostructures of various morphologies including, nanospheres, nanorods, nanowires, nanoprisms, nanoplates and branched nanostructures have been synthesized. In this work, we are reporting the formation of various shapes of gold nanoparticle from popular tuberculosis drug INH as a reducing agent. In the my best knowledge, this drug molecule is first time using as reducing agent to the formation of the gold nanoparticles. To achieve various shapes, pH values and different capping agents have been employed. Successful syntheses of gold nanoparticles are confirmed by several techniques such as UV-Vis Spectroscopy, SEM, TEM and Raman Spectroscopy. Oxidation of nicotinamide adenine dinucleotide (NADH) and SERS measurement of many required molecules has been planned to do from these gold nanoparticles.

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Studies of Tungsten, Dysprosium, Barium oxide nanoparticles as CT Contrast Agent

김성준 **Xu Wenlong Badrul Alam Bony tirusew tegafaw MiaoXu Md. Wasi Ahmad** 이강호*

경북대학교 화학과

We have studied for improved contrast agents and found some materials. They were Tungsten, Dysprosium and Barium oxide nanoparticles. So, We synthesized Tungsten oxide, Dysprosium oxide and Barium oxide nanoparticles as CT contrast agent in order to improve contrast. To be used as clinical CT contrast agent, they were coated with D-glucuronic acid which is hydrophilic and biocompatible ligand. They characterized by using MP-XRD, TGA, FT-IR, HRTEM and In vitro cytotoxicity test.

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REMPI, UV-UV Hole-burning and IR dip Spectroscopic Studies of Jet-cooled 5-cyanoindole

이지훈 민아름 안아름 문철주 김성근[1] 최명룡*

경상대학교 화학과 [1]서울대학교 화학부

5-cyanoindole(5-CI) as a derivative of indole has important intrinsic properties for its enormous biological activities in biological systems. We measured the excitation spectra of jet-cooled 5-CI using resonance-enhanced multiphoton ionization (REMPI) in the gas phase. As a result, we obtained sharply congested REMPI spectrum of 5-CI. Then, we identified that 5-CI has one conformer via UV-UV hole-burning and IR dip spectroscopy. Moreover, we also calculated the optimized structure of 5-CI by density functional theory (DFT) with a 6-311++G(d,p) basis set. Here, we report the structural information of 5-CI by comparing the each experimental data and from the theory.

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A study of Photophysical property of Nanosized graphene oxide

최종완 김낙중*

한양대학교 화학과

Graphene has been receiving much attraction in various research fields due to exceptional physical and photonic properties. Furthermore of Nanosized graphene can be good for making optoelectronic device, sensor, and bioimaging application that has strong and stable photoluminescence, excellent solubility, and low cytotoxicity. Several studies of band gap tuning or photoluminescence shifting of nanosized graphene (or graphene oxide) have investigated. In this work, we prepared nanosized graphene oxide and reduced graphene oxide through hydrothermal reaction. And we also controlled band gap of nanosized graphene oxide by chemical functionalization. The nanosized graphene oxide was characterized by FT-IR, UV-Vis and photoluminescence spectra, AFM, and TEM.

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Catalytic Reductive Dechlorination of 1,1,1-trichloro-2,2-bis(4-chlorophenyl)ethane (4,4'-DDT) using Bimetallic Iron-Palladium Nanoparticles Produced by Pulsed Laser Ablation in Liquid(PLAL)

제민규 이슬기 정현진 최명룡*

경상대학교 화학과

Persistent organic pollutants (POPs) have concerned public due to their toxicity, bioaccumulation and persistency in the environment and human health. Bimetallic catalysts have recently appeared significant effect for the remediation of groundwater and sediment contaminated with chlorinated organic compounds. Fe nanoparticles were produced by pulsed Nd:YAG laser (1064nm, 10Hz, 7ns) ablating onto an Fe plate immersed in methanol with a reducing agent, ascorbic acid. The morphological and optical properties of Fe/Pd catalysts via PLAL were characterized by transmission electron microscopy (TEM), X-ray diffraction (XRD), Ultraviolet-visible spectroscopy (UV-Vis). Fe/Pd catalysts were used to the dechlorination of 4,4’-DDT under various conditions. The products of dechlorination reactions were analyzed by gas chromatography (GC). This study suggested that Fe/Pd catalysts could be potentially employed to rapidly degrade 4,4’-DDT in the contaminated environment.

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Specific solvents produce specific phase Ni nanoparticles via pulsed laser ablation in solvents

정현진 최명룡*

경상대학교 화학과

We report a simple and controllable preparation of face centered cubic (fcc) and hexagonal close-packed (hcp) Ni nanoparticles by a pulsed Nd-YAG laser ablation method in various solvents, such as deionized water, methanol, hexane, and acetonitrile. We generate Ni/NiO and fcc/hcp Ni nanoparticles by a laser ablation to a Ni plate submerged in various solvents, followed by a post-ablation to the colloidal solutions. Interestingly, the phases of Ni nanoparticles prepared via PLAL show a strong dependence on the solvents used in the ablation process. Ni/NiO, pure fcc, and mixture of fcc and hcp Ni nanoparticles were generated in DI water, methanol, and hexane or acetonitrile, respectively. After the post-ablation, however, pure fcc Ni nanoparticles were generated in methanol and hexane; while pure hcp Ni was formed in acetonitrile. We think that the solvent dependence on the phase of Ni nanocrystals is related to the specific heat of solvents that plays an important role kinetically and thermodynamically in the process of cooling the plasma plume where the nanoparticles nucleate and coalesce to a specific phase. Formation of graphite layers on Ni nanoparticles fabricated in hexane and acetonitrile is also discussed. The Ni nanoparticles prepared from PLAL were analyzed by X-ray diffraction (XRD) measurements, X-ray photoelectron spectroscopy (XPS), field emission scanning electron microscopy (FE-SEM), high resolution transmission electron microscopy (HRTEM), and fast Fourier transform (FFT) analysis.

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Excited-state dynamics of DCM near plasmonic nanoparticles

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광주과학기술원(GIST) 물리화학부

Ultrafast transient absorption measurements in visible wavelengths have been used to investigate the excited-state dynamics of 4-(dicyanomethylene)-2-methyl-6-(4-dimethylaminostyryl)-4H-pyran (DCM) in methanol near a silver island film. Transient absorption spectra of DCM in methanol with the silver surface are very similar to those of free DCM without the silver surface. However, kinetics of stimulated emission bands arising from the charge-transferred S1 state show a rise component of ~30 ps with the silver surface which was absent in the free DCM case. They also show a longer (~2.0 ns) lifetime of the S1 state with the silver surface compared to the value (~1.5 ns) of free DCM. These results support the idea of the ultrafast energy transfer from silver nanoparticles to DCM molecules.

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Morphology-controlled synthesis of twinned structural ZnO crystals and their antibacterial activities

진다혜 조영식 허영덕*

단국대학교 화학과

Various twinned morphologies of ZnO were prepared from $CuCl_2$, N,N'-Dimethyl ethylenediamine (DMEDA) and sodium 1-heptanesulfonate with a hydrothermal reaction. DMEDA and sodium 1-heptanesulfonate were used as the hydroxide ion generator and the morphology controller, respectively. As the sodium 1-heptanesulfonate concentration increases, the twinned structure of ZnO product changes from thin hexagonal rods with bipyramidal ends to thick hexagonal plates. The ratio of the (001) polar plane to the (110) nonpolar plane of ZnO also increases with the concentration of sodium 1-heptanesulfonate. We also investigates the antibacterial activity of these ZnO crystals. The polar character of the (001) plane plays an important role in the antibacterial activity.

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PAA를 포함한 PMMA 아이오노머의 동적 기계적 성질

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조선대학교 신재생에너지융합학과 [1]조선대학교 첨단부품소재공학과 [2]조선대학교 화학교육과 [3]조선대학교 응용화학소재공학과

PMMA 아이오노머에 저분자량의 PAA 를 첨가하였을때 가소제 또는 충진제의 성질을 보이는지에 대한 연구를 하였다. PMMA 아이오노머에 PAA 를 각각 무게비로 10wt%, 5wt%, 3wt%로 첨가하여 PMMA 아이오노머에 PAA 의 함량이 어떠한 영향을 미치는지 DMA 를 이용하여 동적 기계적 성질을 측정하였다. PAA 의 함량이 증가 할수록 PMMA 아이오노머의 loss tangent peak 의 크기가 작아지고 ionic modulus 값은 증가함을 알 수 있었다. 그러나 PAA 의 함량이 변해도 PMMA 아이오노머의 matrix T_g는 변하지 않았다.

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S2 Fluorescence Dynamics of meso-Aryl-substituted Subporphyrins

성주영 김동호*

연세대학교 화학과

In contrast to the porphyrin case, little is known about the photophysical behaviour of subporphyrins, and up until now, observation of their S2-fluorescence has never been reported. Hence, information regarding the higher excited states of subporphyrins is of great interest in their own right, which will shed light on an in-depth understanding of the nature of electronic excited state of subporphyrins. We have demonstrated the first direct observation of S2-fluorescence of subporphyrin. Besides S1 fluorescence, another fluorescence band was observed for subporphyrin upon excitation at the respective Soret-like band. This fluorescence spectrum has been assigned as S2 fluorescence on the basis of their mirror images of the S2-S0 absorption. We find that a distinct structural feature of the subporphyrin (i.e., domed structure) increases the density of vibronic states which may play an important role in shortening the excited S2-state lifetime of subporphyrin relative to ZnTPP (i.e., planar structure) and hence, accelerate the S2-S1 internal conversion process. However, interestingly, based on our observation of the anisotropy in the higher excited states of subporphyrin, it is inferred that the two transition dipoles of degenerate S2-states are orthogonally oriented despite the C3 symmetry of molecules. This study has successfully identified fundamental photophysical properties and higher excited-state relaxation dynamics of subporphyrins. Therefore, we think that these findings not only give an insight into the future experimental and theoretical study of subporphyrins but also pave the way for the use of subporphyrinoid systems in the fields of molecular materials.

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Ultrafast Dynamics of Nitroxyl Myoglobin (Mb-DNO) by Femtosecond Vibrational Spectroscopy

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부산대학교 화학과 [1]부산대학교 나노메디컬공학과

Nitroxyl (HNO), a reduced form of NO, plays many important biological roles. Free HNO forms dimer which decomposes into nitrous oxide and water in solution but HNO binds to ferrous heme proteins to form stable HNO-bound heme adduct. Though many experimental and theoretical researches for nitroxyl myoglobin (MbHNO) were performed to identify its active site structure, photophysical and photochemical process of MbHNO have not been fully understood yet. We used femtosecond pump-probe vibrational spectroscopy to probe photoexcitation dynamics of MbDNO with a 575 nm pulse. Three vibrational bands at 1365, 1375, and 1399 cm^{-1} were observed for the N?O stretching mode related vibration. Based on absorption band of the MbD^{15}NO and ab initio calculations of DNO-bound model heme, the three absorption bands were attributed to Fermi interaction of the N-O stretching mode and weak combination and overtone modes of the N-related vibration. Transient bleach appears instantaneously and about 92% of it decays in 4 ps, indicating that DNO is photodeligated immediately upon photoexcitation of MbDNO and most of the deligated DNO rebinds to Mb efficiently.

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Photophysical Properties of Cyclic Perylene Bisimide (PBI) Trimer Probed by Single-Molecule Fluorescence Spectroscopy at Low Temperature

김태우 김동호*

연세대학교 화학과

Single-molecule spectroscopic techniques have become powerful tools for investigating the photophysical properties of the molecular systems by overcoming the limitations of ensemble measurements which offer only the simple average phenomena. Moreover, at low temperature, it is possible to observe the characteristics of the single molecule much clearly from fluorescence spectra which allow us to distinguish several emitting sites due to decreased thermal broadening.We have studied the photophysical properties of cyclic PBI trimer (C3) by measuring fluorescence intensity trajectories (FITs), fluorescence spectra and fluorescence lifetimes. Fluorescence spectra and fluorescence lifetimes were constructed by fluorescence photons at each emissive level in the FITs. As fluorescence intensity changes step by step, the fluorescence lifetime and spectral peak position slightly change. This feature suggests that the interaction among the PBI units in C3 is very weak so they act as an individual chromophore as reported in our earlier ensemble and single-molecule level study at room temperature. Moreover, we observed different emitting states in single C3 molecule from fluorescence spectra, which cannot be seen at room temperature due to similar energy levels in each chromophore of C3 and broadening effect.In addition, we are planning to perform the single-molecule fluorescence spectroscopy at low temperature with cyclic PBI hexamer (C6) which shows more distorted structure than C3. We expect that we can observe more complicated phenomena in C6, and futher these results will provide detailed informatioin on the structure-property relationship depending on molecular structures.

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Rebinding dynamics of CO bound to Cytoglobin in D_2O

김주영 임만호* **Hitomi Sawai[1]**

부산대학교 화학과 [1]RIKEN SPring-8 Center

Cytoglobin, a heme-containing protein, was found in vertebrates. It is found in a wide range of mammalian tissues and is also available to bind with external ligands. Unlike myoglobin Fe in heme plane of Cgb is six coordinated with distal and proximal histidine. In this study, We measured the rebinding dynamics of the CO complex of Cytoglobin in aqueous solution using femtosecond and nanosecond vibrational spectroscopy.

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FT-IR studies of electrolyte aqueous solutions

임준형 조민행*

고려대학교 화학과

Recently, there is a growing interest in understanding the connection between the water structure and dynamics and biolchemical mechanisms in cells. Watterson et.al[1] and Pollack et.al[2] showed that water network dynamics can affect protein structure and its functionality. In this presentation we show the study of water structure in aqueous solutions of simple salts investigated in terms of fourier transform infrared spectroscopy (FT-IR). This technique is selected because of the sensitivity of virbrational lineshape and position to environmental changes around the vibrational probe. Here, we investigate the correlations between OD stretch band features with the nature of cation and anions. References[1] Watterson, J. G. (1997). The pressure pixel?unit of life? Biosystems 41, 141-152[2] Pollack, G. H., and Reitz, F. B. (2001). Phase transitions and molecular motion in the cell. CellMol. Biol. 47, 885?900.

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Raman Investigation of Heterogeneity from Partially Grown Graphene

구은혜 주상용*

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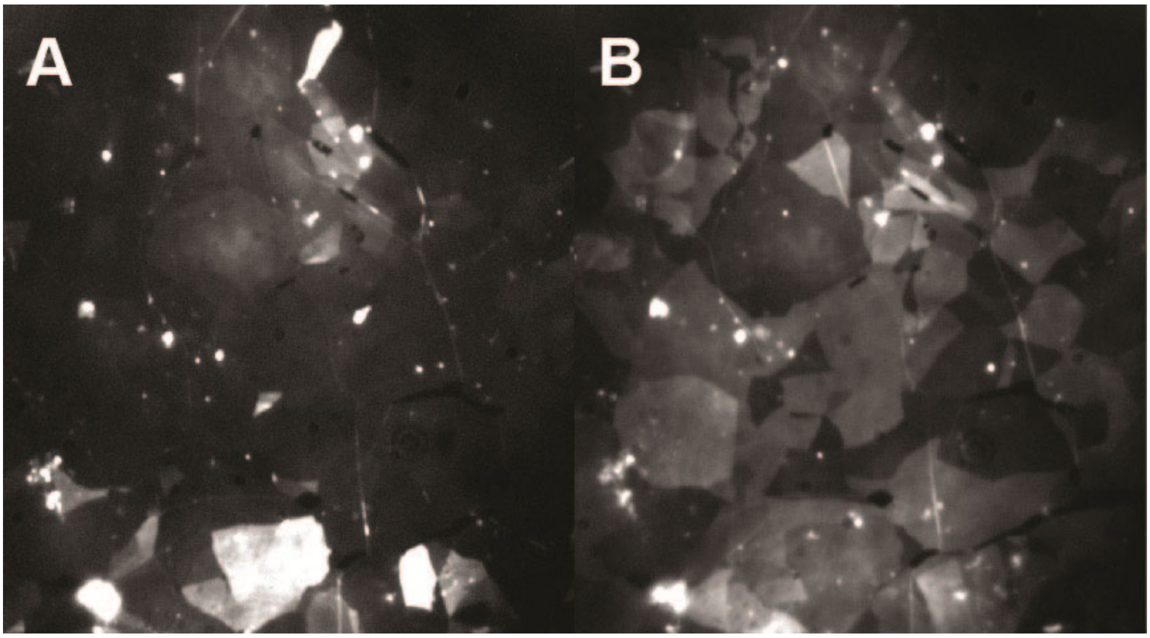
Recently, Chemical vapor deposition (CVD) method is actively used for graphene synthesis. Due to the fact that CVD grown graphene has a difficulty in electrical applications as compared to mechanically exfoliated graphene, it is desirable to investigate initial grains of CVD graphene to overcome its limitation. Heterogeneity of CVD grown graphene is detected using widefield Raman spectroscopy, which is originated from doping, defect density, stacking order, rotation angle dependency and number of layers. We observe doping induced from substrate and polymethyl methacrylate(PMMA) residues. Suspended graphene shows downshifted position and band broadening of G and 2D bands compared with substrate-supported graphene. In the case of PMMA covered grain, position of G band increases and 2D band is downshifted, along with band broadening. As defect density gradually increases, positions of G and 2D bands are upshifted and their band-broadening occurs. Rotationally stacked bilayer graphene shows distinctive Raman features as compared to Bernal(AB) stacked bilayer graphene. Depending on the rotation angle, R and R’ peaks which are originated from inter- and intra-valley double resonance processes appear. Besides, specific patch of grain shows enhanced G band along with narrower 2D band. This study provides systematic standards to understand properties of CVD grown graphene.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Time dependent vibrational predissociation of AnWn cluster cation

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경희대학교 화학과

AnWn+ clusters generated by doubling of visible OPO output signal in the range 440-600 nm. Mass selected ions are dissociated applying field potential (3000-2000V) with infrared (IR) to analyze the rate of dissociation. Variation in the wavelength for ionization will change the internal energy of the parent ion. Dependence of the energy applied for ionization on the rate of predissociation is the main goal of this research. For any known system the increase in internal energy, increases the rate of dissociation, but for larger cluster it is hard to see this trend. So to investigate the actual dependence of rate constant on cluster predissociation this research may give some further idea to the chemist.

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Dynamics of laser ablation in liquid phase : the effect of magnetic field and electrolyte

김국기 **Madhusudan Roy** 송재규 박승민*

경희대학교 화학과

We investigated the effect of magnetic field and electrolyte on the plasma plume produced by laser ablation of metal in water. We found the optical intensity of plasma plume depends on laser power, magnetic field and electrolyte. Liquid-phase plasma plume analyzed by intensified charge coupled device (ICCD). Also we have studied laser-light scattering for growth processes of silver nanoparticles in liquid phase laser ablation.

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Fabrication and Photocatalytic Property of TiO2 Based Multicomponent Nanocomposites

임지은 **LIJING** 김용록*

연세대학교 화학과

Titanium dioxide(TiO2) has widely used in photocatalysis because of its high photocatalytic activity and durability. Many researches have been performed to enhance photocatalytic efficiency of TiO2. In this study, we synthesized porous TiO2-based multicomponent nanocomposites. The morphology was characterized by SEM, TEM, XRD and BET. The photophysical properties of the TiO2-based multicomponent nanocomposites were characterized by UV?Vis spectrophotometer and spectrofluorometer. The fabricated TiO2-based multicomponent nanocomposites photocatalysts are improved visible-light photocatalytic activity due to their large surface area and wide range of absorption spectra.

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Effects of laser wavelength and energy density in Ni nanoparticles by pulsed laser ablation in deionized water using a surfactant, SDS

마로리 김태규*

부산대학교 화학과

Nanoparticles (NPs), the nano-scale metal particles, have unique properties different from bulk material because of its quantum effect which causes their new magnetic, electronic, optical, and thermal properties. Specially, metal nanoparticles are successfully used in a wide range of applications like catalysis, sensing, capacity and so on. There are many methods to synthesize NPs. One of methods is pulsed laser ablation in liquid (PLAL) which is attractive methods to produce metal NPs in the past decade. In this experiment, we use a pulsed nanosecond Nd: YAG laser in deionized water with Ni plate with or without 0.01 M surfactant of sodium dodecyl sulfate (SDS). This experiment is performed to irradiate laser focused on Ni plate in SDS solution during 60 min. It produces NiO NPs at different laser wavelength (532 nm, 1064 nm). Energy density (3.2 J/cm2, 10.5 J/cm2 and 19.9 J/cm2) are changed to control the beam diameter. Laser power is fixed by 100 mJ/ pulse. In this study, the mean diameter and width of size distribution of NiO NPs are affected by wavelength and laser energy density. This experiment also shows a role of surfactant, SDS, in PLAL that is to make NPs size be uniform distribution. In addition, structural and morphological characterizations of synthesized NiO NPs are conducted by cyclic voltammetry (CV) using multi-walled carbon nanotube (MWCNT) to synthesize NiO/ CNT composites, UV-vis spectroscopy and high resolution transmission electron microscopy (HR-TEM).

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Non-universal Dynamic Behavior in Two Dimensional Random Obstacle Matrices

조현우 성봉준*

서강대학교 화학과

The random obstacle matrices have been employed extensively for studying anomalous dynamic behavior of the spatially heterogeneous environment, such as cell cytoplasm, cell membrane, or colloidal glass. The tracer diffusion constant in the random obstacle matrices, D, follows the scaling relation, i.e., $D\sim(\varphi-\varphi_c)^{\mu}$, where φ is the density of the obstacles, φ_c is the value of φ at the percolation threshold, and μ is the dynamic scaling constant. It has been believed that the exponent μ should be a universal quantity in two dimensions, i.e., μ should depend not on system details. In this work, however, we show that μ should be non-universal even in two dimensions, and elucidate the physical origin of such non-universality. We put the tracers on the two dimensional random obstacle matrices, and obtain the value of D using the dynamic Monte Carlo simulation. According to our simulation result, μ increases with an increase of the maximum displacement for the translational motion of the tracer, Δ. We discretize the void space into triangular cells using Delaunay tessellation, and evaluate the transition rate of each triangular cell, W. Interestingly, as Δ increases, the distribution of W becomes singular at the origin, which makes the value of μ non-universal. We also discuss our simulation results in comparison with renormalization group theory.

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Two Emissive States in the Excited State of Thioflavin T

김준우 주태하*

포항공과대학교 화학과

Thioflavin T (ThT) is a molecular probe to observe amyloid fibrillation. Its fluorescence quantum yield increases dramatically when it is in rigid environment, such as viscous solvent or fiber. The molecular structure of ThT (Fig. 1 (a)) composes of aniline and thiazole group. Previous researches suggest that the two groups are twisted at the equilibrium configuration of the excited state, and the fluorescence enhancement is caused by the restriction of the twisting. However, there are no explicit evidences for the twisted configuration. Here we have measured the time-resolved fluorescence (TRF) with 55 fs resolution, and interpreted the excited-state dynamics of ThT by coherent nuclear wave-packet analysis. We obtained a twisted and a planar structure in the excited state in water and vacuum respectively. Those are calculated by TD-DFT method at cam-B3LYP/6-311G(d) level with the polarized continuum model. The normal mode projection data from the two structures to the ground-state configuration, and the oscillation components extracted from TRF data are represented in Fig. 1 (b). The vibrational motion of 77 cm-1 of the twisted configuration shows twisting motion and detected only TRF at 510 nm. In contrast, the motions around 180 cm-1 of the planar structure are associated to bending motion were detected in TRFs at 460 and 610 nm. As a result, there must be two emissive states and one of them is twisted, and the other is planar.

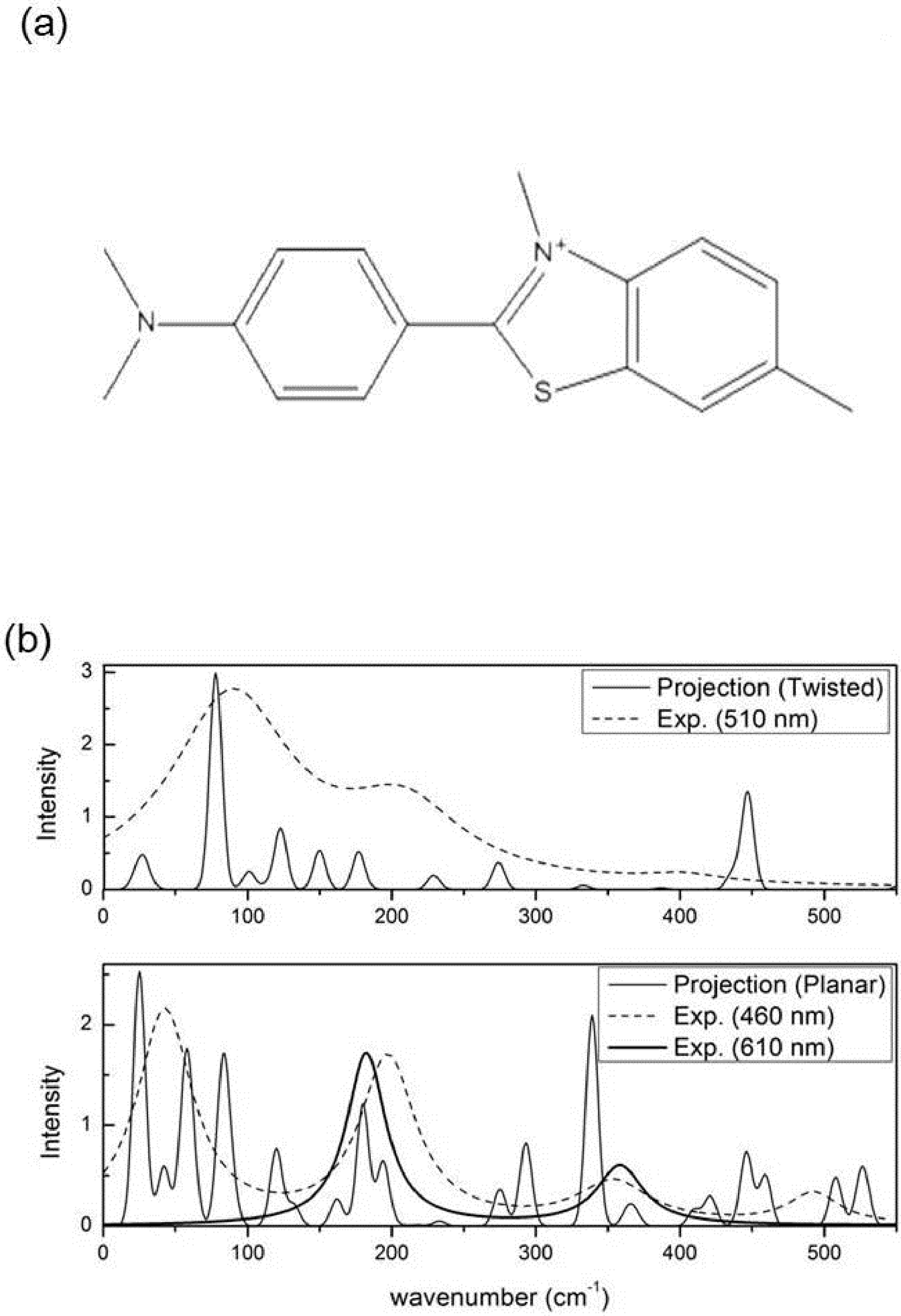

Fig. 1 The molecular structure of Thioflavin T (a), and the oscillation components in frequency domain from LPSVD analysis (b). For comparison, the normal mode projection data from the twisted (top, solid) and the planar (bottom, solid) configuration of excited state ThT with relative amplitude is represented.


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A simulation study on rotational dynamics in 2-dimensional heterogeneous environments

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Porous media has been a subject of significant academic interest, especially from a theoretical standpoint. When the volume fraction (φ) of matrix molecules is sufficiently high, the system becomes significantly heterogeneous, thus resulting in anomalous transport behaviors of tracer molecules in porous media: tracer molecules show anomalous sub-diffusion at a certain time scales and undergo hopping motions. Because transport of tracer molecules in porous media is related closely to various applications such as gel electrophoresis, protein diffusion in cell membranes, and gas permeation membranes, there have been extensive theoretical and experiment studies on the translational diffusion of tracer molecules in porous media. There have been few studies, however, on the rotational dynamics of tracer molecules in porous media. In this study, we employ molecular dynamics simulations to investigate the tracer dimers in porous media and find that tracer dimers also show very interesting dynamic behaviors. When there is a percolating network of pores in porous media, tracer dimers show normal rotational diffusion with the self-part of van Hove angular distribution functions ($G_s(\theta,t)$) being of a Gaussian shape. When the percolating network disappears at a sufficiently high φ, the rotational diffusion is still seemingly Brownian but with exponential and/or oscillatory $G_s(\theta,t)$. We investigate trajectories of each dimer and find that the rotational dynamics of a single dimer should be strongly influenced by the local environment of porous media, which results in the anomalous oscillatory space-time correlation functions ($G_s(\theta,t)$).

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Dynamic Decoupling and Glass-Forming Ability of Multicomponent Bulk Metallic Glasses

김정민 성봉준*

서강대학교 화학과

Bulk metallic glasses (BMGs) have drawn significant attention because of their promising mechanical properties. Sufficiently fast supercooling of multicomponent alloys prevents a transformation of the alloys to solids, and enables BMGs to be formed. Thus, glass-forming ability (GFA) of BMGs is inversely related to the critical cooling rates. Interesting dynamic feature of BMGs is dynamic decoupling, such as breakdown of Stokes-Einstein relation (SER), which has been intensively studied to understand fundamentals of the glass transition. The dynamic decoupling of BMGs is also related to their GFA. For example, a glass-forming $Pd_{43}Cu_{27}Ni_{10}P_{20}$ alloy shows a strong component decoupling of diffusivities between the largest component Pd atom and others when the alloy is supercooled below a critical temperature [1]. The component decoupling of different species may be responsible for the excellent GFA of the alloy. To elucidate the relation between the dynamic decoupling and the GFA, we carry out molecular dynamics simulations for hard sphere mixtures modeled after $Pd_{43}Cu_{27}Ni_{10}P_{20}$ melts. We find out that SER starts to break down at a critical volume fraction. Near the critical volume fraction, component decoupling is shown with dynamically heterogeneous P, and immobile Pd which forms slow subsets. Moreover, we show that the excellent GFA of the alloy may also stem from dynamically heterogeneous P, disrupting formation of crystal nuclei.Reference[1] A. Bartsch et al., Phys. Rev. Lett. 104, 195901 (2010)

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Photodissociation dynamics of Bromocyclohexane near 234nm : Ion imaging study

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부산대학교 화학과

The Photodissociation dynamics of bromocyclohexane have been investigated near 234nm using a velocity map imaging (VMI) technique coupled with state selective [2+1] resonance-enhanced multiphoton ionization (REMPI) scheme. REMPI scheme was used for state-selective detections of Br and Br* generated after photodissociation of bromocyclohexane near 234nm. Using REMPI scheme, we can monitor specific state at specific wavelength. Result of our work, we get the raw image. In case of excited state, it consists of two rings. However, ground state has just one ring. For more detail information, we analyzed these images. we measured total translational energy distributions, recoil anisotropic parameters, and the relative quantum yields. There translational energy distribution is can fitted by two Gaussian functions at both state. The experimental result also showed that Br formation is dominant with the relative quantum yield 0.81 near 234nm.

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단백질응집반응의 이해와 조절에 대한 연구

한상훈 김호태*

금오공과대학교 응용화학과

본 실험은 monomer(YGGFL, NFGAIL, VEALYL)를 이용하여 oligomer의 형성과정을 알아보고 단백질에서의 응집 반응에 대하여 확인하고자 하는 실험이다. 또한 Cu 이온과 oligomer 와의 상호작용을 통해서 일반적인 응집 반응과 어떤 차이가 발생하는지를 확인하고자 한다. ESI Mass Spectrometer 를 이용하여 oligomer 의 형성 여부를 확인하고, MS 와 MS/MS 실험을 진행하여 어느 부분에서 oligomer 의 결합이 형성된 것인지 확인하고자 하였다. Computation 을 이용하여 에너지와 구조를 계산하고, 실험에서 관측된 fragmentation pattern 을 설명하고자 하였다.

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Exploring size and composition dependent exciton relaxation in PbS and PbSe using hyperspectral near IR probing

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연세대학교 화학과 [1]한국기계연구원 나노기계연구본부

We conduct hyperspectral femtosecond transient absorption measurement to record exciton relaxation process of lead chalcogenide (PbS and PbSe) nanocrystal quantum dots (NQDs) as a function of excitation energy (ħω) and power. It has been reported, for NCs in such a small size regime, a large percentage of the atoms is on or near the Surfaces. Vast interface between the NC and the surrounding medium can have a profound effect on the NC properties because imperfect surfaces act as electron and hole traps upon optical excitation. In addition to the differences in the properties of the NQD surface and/or the number and identity of external acceptor trap sites, the effect of the NQD size is defined as the quantum confinement energy. Second derivative analysis of the absorption spectra was employed to clearly identify transitions and the dependence of their quantum confinement energy on the size of the NCs.

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DYNAMIC MECHANICAL PROPERTIES AND MORPHPLOGY OF SODIUM NEUTRALIZED PSMA IONOMERS CONTAINING VARIOUS DIMER ACID

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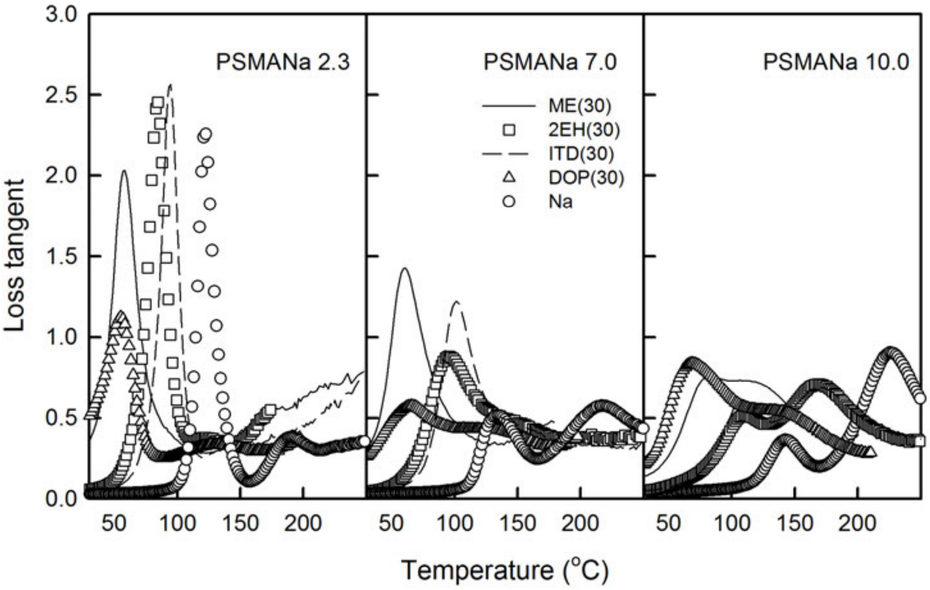
조선대학교 첨단부품소재공학과 [1]조선대학교 화학교육과 [2]조선대학교 신재생에너지융합학과 [3]조선대학교 응용화학소재공학과

The effects of the addtion of various dimer acid(DA) on the dynamic mechanical and thermal properties and morphology of poly(styrene-co-sodium methacrylate)(PS-co-MA)Na ionomers were studied using DMA, TGA, SAXS and XRD techniques. The methacrylic acid contents were found to be 2.3, 7.0, 10.0 mol%. The mechanical properties and morphology of ionomers containing dioctyl phthalate(DOP) were also studied and compared to those of DA-containing ionomers. In the case of the ionomer containing the ME at the same ion content, the positions of loss tangent peaks shifted to lower temperature. The same was true for the ionomer containing DOP. The effectiveness of plasticization is in the following order: DOP ≥ ME > 2EH ≥ ITD.



3.0
2.5
2.0
1.5
1.0
0.5
0.0
Loss tangent
PSMANa 2.3
PSMANa 7.0
PSMANa 10.0
ME(30)
2EH(30)
ITD(30)
DOP(30)
Na
50
100
150
200
Temperature (°C)

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Theoretical Study for Chemisorption and Associative Desorption of Hydrogen on Graphene

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경희대학교 응용화학과

그래핀은 탄소 원자 6 각형으로 이루어진 aromatic conjugation 구조이며 띄어난 전기전도성과 화학적 성질을 가지고 있다. 두 층의 그래핀은 π-π interaction 에 의해 다른 전기적, 화학적 성질을 갖는다. 본 연구는 하나의 수소 원자가 첨가된 sp^3 그래핀의 반응속도가 π-π interaction 에 의해 어떠한 영향을 받는지 알아보았다. 그래핀과 수소 원자의 화학반응에는 화학흡착반응 의외에 연합이탈 반응이 있을 수 있다. 경쟁반응으로써 그래핀에 수소 원자 첨가에 따른 화학흡착반응을 연합이탈 반응과 비교하여 관찰하였다. 반응동역학 계산은 Density functional theory 를 사용하여 Potenrial surface energy 를 계산하였고, 다차원 터널링 근사를 고려한 변분법적 전이상태이론을 이용하여 반응속도상수와 터널링 효과를 연구하였다. 단 층의 그래핀과 두 층의 그래핀은 반응 장벽 에너지가 유사하게 나왔다. 터널링 상수는 π-π interaction 이 C-H stretching 진동에 영향을 주어 298K 에서 단 층의 그래핀이 4.3 이며 두 층의 그래핀이 4.1 으로 단층의 그래핀에서 큰 것을 알 수 있었다.

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Fabrication and Characterization of Photofunctional Metal Alloy for Bio-applications

허일 왕강균 김용록*

연세대학교 화학과

Stainless steel is a type of metallic alloy that has been used as a biomaterial for human applications. Among various metal alloys, stainless steel has several advantages for the applications. It has good wear resistance, crevice corrosion resistance, and pitting resistance. In this study, we fabricated photofunctional stainless steel for bio-application. Photophysical properties of the photofunctional stainless steel were studied by steady-state absorption and emission spectroscopies and the photocatalytic effect was evaluated by using conventional organic decomposition reaction. For the feasibility of its bio-application, in particular, as an antimicrobial system, the photofunctional stainless steel was applied to the removal of harmful microorganism.

Acknowledgement
This work has been collaborates with *Prof. Seok Hoon Jung* in Yonsei university, college of medicine.

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Fabrication and Characterization of Photofunctional Polymer For Bio-Applications

황정욱 왕강균 정승진 김용록*

연세대학교 화학과

Reactive oxygen species (ROS) that are commonly associated with photodynamic inactivation (PDI) has been applied to the sterilization of medical instrument and drinking water contaminated by bacteria, viruses, yeasts, and parasites. In this study, we report fabrication of the photofunctional polymer and their photophysical properties estimated with various spectroscopic methods such as steady-state absorption/emission spectroscopy and time & wavelength-resolved phosphorescence spectroscopy. For possibility of bio-application, the fabricated photofunctional polymer was applied for elimination of health hazards. Acknowledgement: This work has been collaborates with *Prof. Seok Hoon Jung* in Yonsei university, college of medicine.

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Electronic Circular Dichroism Spectroscopy of ephedrine and pseudoephedrine in a supersonic jet

홍아람 김남준*

충북대학교 화학과

Circular dichroism (CD) spectroscopy has been a powerful tool to reveal molecular configurations and structural changes of chiral molecules in chemical and biological reactions. However, most CD spectroscopy has been performed in condensed phase and a few research groups have investigated the CD spectra of gaseous chiral molecules. CD spectroscopy of cold molecules in the gas phase is a promising technique because it is possible to reveal absolute configurations of molecules in the gas phase. Recently, we have obtained the first resonant two-photon ionization (R2PI) CD spectra of ephedrine and pseudoephedrine stereoisomers produced in a supersonic jet using circularly polarized nanosecond laser pulses generated through a photoelastic modulator. The spectra of pseudoephedrine exhibit well-resolved CD bands for the origin bands of three different conformers, one of which has the opposite CD sign to the others of the same chirality. This spectral feature is well reproduced by theoretical calculations using the time-dependent density functional theory. From this result, we found that the CD spectroscopy is selective not only to enantiomers but also to conformational isomers.

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Prediction of the effects of amino acid substitutions on Arabinose binding protein

김철희 김은애*

조선대학교 약학과

L-Arabinose isomerase (AI) catalyzes the isomerization of L-arabinose to L-ribulose. The enzyme required divalent metal ion, Mn2+ for enzymatic activity and thermostability improvement at higher temperature. The optimal temperature of the activity is about 70 ℃. The current study describes the optimized structure of the enzyme protein and the enzyme-ligand complex at 20 ℃ and 60 ℃ using molecular dynamics (MD) simulation. Compared with X-ray structure, the conformational change is the out-of-plane bending of the α-helix region from Leu19 to Ser43 sequences. We focused on the binding site open of the enzyme and tried the mutation study for finding the driving force of the mechanism. For more detail opening mechanism, Tyr20 is replaced by other amino acid such as Phe and Ala. We also elucidate the effects of amino acid substitution on the enzyme.

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한약재 추출물의 활성산소종에 대한 항산화 특성 연구

김다솜 안태규*

성균관대학교 에너지과학과

다양한 한약재에 대한 항산화효과를 분광학적 방법으로 고찰하였다. 한약재의 종류로는 금문대황, 녹차, 연교, 황백, 지실등이고 비교시료로 비타민 C 를 측정하였다. 측정결과로 지실이 월등히 좋은 항산화 효과를 보여주었으며 나머지는 각각 황백, 비타민 C, 연교, 녹차, 금문대황의 순서로 나타났다. 가장 효과가 낮은 금문대황의 경우에는 과량의 주입에서도 전혀 항산화 경향을 나타내지 않았다. 또한 단일항 산소의 분광학적인 직접적인 증거를 고찰하였다.

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New mapping of photosynthetic efficiency from geostationary satellite

김다솜 안태규*

성균관대학교 에너지과학과

Photosynthesis of plants can measure quantum yield by the intensity of fluorescence. We made a photosynthetic efficiency map of Korean by using image from geostationary satelite. In addition, we had been studying a lot of application related to yield of photosynthesis.

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Synthesis of push-pull structured organic small molecules as a donor for organic solar cells

박다솜 이진호 장성연* 임상규*

국민대학교 생명나노화학과

Design and synthesis of photoactive materials with appropriate band gap and charge transport properties are a crucial issue in developing high performance organic solar cells (OSCs). To reduce the band-gap of the photoactive molecules, the “push-pull” structure has been widely suggested as an effective strategy. In this work, we synthesized “push-pull” structured organic p-type donor molecules for the photoactive materials OSCs. The molecules contained benzo[1,2-b:4,5-b']dithiophene as a push part, bithophene as a conjugated moiety, and the dicyanovinyl as a acceptor part. The band-gap and molar extinction coefficient were measured using UV-vis spectroscopy. Bulk heterojunction (BHJ) structure of organic molecules and C60 was fabricated by an organic molecules beam deposition method, and used as the active layers. The OSCs using these active layers exhibited the power conversion efficiency of 1.49%.

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The Concentration Effects of PEO on the Interaction of PEO with SDS

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강릉원주대학교 화학과

계면활성제와 고분자간의 혼합물은 독특한 특성을 가지고 있어 학문적, 산업적으로 널리 사용되고 있다. 계면활성제에 고분자의 첨가는 이들 사이의 강한 정전기적 및 소수성 상호작용으로 인하여 계면활성제만의 CMC(critical micelle concentration) 보다 저 농도에서 마이셀을 형성하는데, 이 이유는 고분자 사슬들이 계면활성제에 흡착하여 마이셀을 형성했기 때문이다. 이와 같은 경우를 CMC 와 구분하기 위하여 CAC(critical aggregation concentration)라 부른다. 또한, 계면활성제의 고농도 부분에서 계면활성제의 마이셀 형성 농도를 C2 라 부른다. 본 연구에서는 음이온 계면활성제인 SDS(Sodium dodecyl sulfate)에 다양한 농도의 PEO(polyethylene oxide)를 첨가함으로써 SDS 의 농도에 따른 PEO 의 반응을 점도, 표면장력, 전도도 측정 방법을 이용하여 살펴봄으로써 PEO 의 농도가 CAC 및 C2 형성에 미치는 영향을 알아보고자 한다.

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Computational mechanistic study about Glucose-to-Fructose isomerization in aqueous media

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Several mechanistic studies of glucose-to-fructose isomerization reaction have been reported and many different reaction pathways have been suggested. Herein, the mechanisms of glucose-to-fructose isomerization in aqueous media enabled by homogeneous catalysts by using computational studies is reported. Calculations show that [1,2]-hydride shift step can be accelerated by water molecule.

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Theoretical Study for Geometric Structures and Characteristic of Cyclic Polythiophene Derivatives

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경상대학교 화학교육과 [1]경상대학교 화학과

Cyclic polythiophene derivatives [(-SC4H2-CC-)n], their derivatives substituted with the functional group (-NH2, -CONH2, -COOH), and their complexes combined with some carbon dioxides were optimized at the HF/3-21G* levels. Geometric structures, bond lengths, atomic charges, HOMO-LUMO energy gaps, and binding energy (BE) were analyzed. With increasing n ($4 \leq n \leq 12$), the structures of the derivatives turn to be planar and HOMO-LUMO energy gap (ΔEH-L) gradually decrease. At $n \geq 14$, the structures of the derivatives curved with varying curvature and the energy gap of HOMO-LUMO (ΔEH-L) increases. In the derivatives with substituted functional group (-NH2, -CONH2, -COOH), the geometric structures are more complex than the corresponding cyclic polythiophene derivatives, respectively. The atomic charges (QS) of the sulfur atom increase : derivative-COOH >derivative-CONH2 >derivative-NH2. The HOMO-LUMO energy gaps (ΔEH-L) of derivative-NH2, derivative-CONH2, derivative-COOH are 8.01~8.57, 7.32~7.56, and 7.67~7.81 eV respectively. The structures of cyclic polythiophene derivatives with the carbon dioxide were optimized through hydrogen bond. Among the complexes, the structure of derivative combined with the carbon dioxide is more stable than the others. The binding energies (BE) of derivative-NH2, derivative-CONH2, derivative-COOH are -1.38 ~ -1.25, -1.51 ~ -1.47, and -1.78 ~ -1.28 eV, respectively.

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CBP에 대한 이론적 연구 : 전하/에너지 이동 및 전하 재결합

고은지 김동욱*

경기대학교 화학과

CBP 는 hole 과 electron 의 수송능력이 뛰어난 물질이기 때문에 OLED 의 host 물질로 흔히 쓰인다. 이 물질의 hole 과 electron 이 어떻게 이동하고 결합하는지 알아보기위해 reorganization energy 와 charge transfer integral 을 계산하였으며 dimer pair 의 charge transfer state 계산을 통해 excited state 를 어떻게 형성하는 지 알아본다.

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Photodynamic Inactivation of Microorganism using Photofunctional Nanocomposite

송형완 신언필 황정욱 왕강균 김용록*

연세대학교 화학과

Nanomaterials have been widely used for bio-application due to long circulation time in the bloodstream and enhanced permeability and retention (EPR) effect. In this study, we fabricated the photofunctional nanocomposite which was then characterized with X-ray diffractometer (XRD), FT-IR spectrometer, UV-vis spectrophotometer, and spectrofluorometer. Photo-functionalities of the nanocomposite were investigated by evaluation of decomposition reaction of organic compounds and time resolved near IR phosphorescence measurement. In addition, it was shown that the photofunctional nanocomposite could be utilized for the removal of harmful microorganism.Acknowledgement.This work has been collaborated with Prof. Chae Seung Lim and Jin Woo Jang (Department of Laboratory Medicine, Korea University).

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Tautomerism of Adenine Complexes with Alkali Metal Cations

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충북대학교 화학과

We obtained ultraviolet (UV) photodissociation (PD) and UV-UV hole burning (HB) spectra of adenine complexed with a potassium cation produced by electrospray ionization (ESI) using quadrupole ion trap reflectron time-of-flight (QIT-reTOF) mass spectrometry. The UV PD spectrum exhibits well-resolved vibronic peaks, which coincide well with those in the UV-UV HB spectrum, indicating the presence of a single isomer in the QIT at ~10K. Although the most stable tautomer of adenine is 9H-adenine (9HA), we found that the most stable adenine complexes with alkali metal cations (M^+A, M=Na and K) in water was M^+7H-adenine (M^+7HA) by theoretical calculation and experimental results on 9-methyladenine and 7-methyladenine complexes with K^+. On the basis of density functional theory calculation on K^+9HA clusters with three water molecules, we suggest that the binding of K^+ ion to 9HA accelerates its tautomerization to 7HA in water by lowering the reaction barrier.

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Synthesis and Characterization of Luminescent Re(III) Complexes with Chelidamic Acid (Re = Eu, Tb, Sm, and Dy)

함아리 강준길*

충남대학교 화학과

Re(III) complexes with chelidamic acid (CDAH3) were prepared and their luminescence properties were investigated for designing highly luminescent Re(III) complexes. The luminescence properties of the complexes were investigated as functions of the molar ration and pH in aqueous states. The maximum intensity of the Re(III) complexes were resulted from the 1:4 Re:CDA molar ration and pH > 10. Single crystals were grown from the optimized solution conditions and their X-ray structures were obtained. Eu(III) and Tb(III) complexes excited at UV light produced very strong red and green luminescence, respectively, by the energy transfer from CDA to Re(III). The barycenter of the energy transfer band was 317 nm.

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Synthesis and Luminescence Properties of Re(III) Complexes with N-benzoylbenzamide and 1,10-Phenanthroline (Re = Eu, Tb, Sm and Dy)

강명현 강준길*

충남대학교 화학과

In this study, we synthesized Re(BBA)3 and K[Re(BBA)4] complexes (Re = Eu, Tb, Sm and Dy, and BBA = N-benzoylbenzamide). The synthesized Re(III) complexes were confirmed with EA, IR and TGA. The Eu(III) and Tb(III) complexes excited at UV produced the strong red and green luminescence, respectively, by the energy transfer (?max = 333 nm) from BBA to Re(III). Only weak luminescence was resulted from the Dy(III) and the Sm(III) complexes. In addition, Re(III) complexes with mixed BBA and 1,10-phenanthroline (phen) in order to investigate the roles of BBA and phen in the sensitized luminescence. It was found that the additional energy transfer (?max = 300 nm) was contributed by introducing phen to the complex.

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Ultrasmall dysprosium manganese oxide nanoparticles as MRI contrast agent

<u>Badrul Alam Bony</u> Xu Wenlong tirusew tegafaw 김성준 MiaoXu Md. Wasi Ahmad 이강호*

경북대학교 화학과

We accomplished a novel and an efficient one-pot synthesis of biocompatible D-glucuronic acid coated ultrasmall $DyMnO_3$ nanoparticles. Aqueous suspensions of nanoparticles were found to possess enhanced r_2 relaxivities and their in vitro studies indicated significant dose-dependent contrast enhancements in T_2 map images indicating them as potential T_2 MRI contrast agents. Remarkable features like high magnetic moment and relaxivities of $DyMnO_3$ nanoparticles were observed. Moreover, the toxicity of $DyMnO_3$ nanoparticles was also minimized compared to MnO/Mn_2O_3 or Dy_2O_3 nanoparticles. The efficiency of D-glucuronic acid coated ultrasmall $DyMnO_3$ nanoparticles as T_2 MRI contrast agent was proved through in vivo T_2 MR Images of a mouse which can be exploited for the rational design of lanthanide based MRI contrast agents.

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Adsorption structures of bicyclic olefin compound on Ge(100)

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대구대학교 화학교육과 [1]한국과학기술원(KAIST) 화학과

The adsorption structures of norbornene on a Ge(100) surface have been investigated using ab initio calculations. The most favorable configuration at low coverage is that the norbornene molecule is bound on top of germanium dimer. Due to the existence of bicyclic moiety, spatial orientation of the norbornene molecule relative to the germanium surface affects the energetic stability of each configuration. The steric hindrance between adsorbed norbornene molecules also affects the adsorption energies of the structures. Theoretical STM images from the relatively stable configuration are consistent with experimentally observed adsorption features.

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Synthesis and Characterization of Water Soluble D-Glucuronic acid coated GdDy Mixed Oxide Nanoparticles

tirusew tegafaw Xu Wenlong Badrul Alam Bony 김성준 MiaoXu Md. Wasi Ahmad 이강호*

경북대학교 화학과

In recent years, magnetic nanoparticle materials have been intensively studied because they often exhibit very interesting properties, which cannot be achieved by their bulk counterparts. Magnetic nanoparticles have drawn tremendous attraction from both fundamental aspect as well as applications in biomedicine such as detection of biological entities, magnetic resonance imaging, magnetic fluid hyperthermia and targeted drug delivery. In this work we synthesized water soluble GdDy mixed oxide nanoparticles with biofunctinalized surface coating. D- glucuronic acid was used for the surface coating of the nanoparticles.The structural, morphological and magnetic properties of these synthesized products were characterized by using X-ray diffraction (XRD), high-resolution transmission electron microscopy (HRTEM), Fourier transform infrared spectroscopy (FTIR), TGA, and SQUID magnetometer.

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Adsorption mechanism of dye molecules on silver and gold nanoparticles studied by surface enhanced Raman spectroscopy

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The surface-enhanced Raman spectroscopy (SERS) of rhodamine dyes (Rh6G, RhB) was investigated by silver and gold nanoparticles synthesized by different reducing agents like borohydride and citrate. Rh6G and RhB show cationic behavior in aqueous solution, so high SERS signal is observed at hotspots formed in nanogaps of flocculated nanoparticles induced by chloride ions even at low concentration (10-8 M) of dye molecules. In rhodamines dyes, xanthene and carboxyphenyl groups possess opposite charges, either of which might attach to the nanoparticles by Coulombic interaction. We have further explored the adsorption mechanism of benzoic acid and related organic molecules to silver nanoparticles. Carboxylic groups of these molecules are mainly responsible for the surface adsorption.

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Developing efficient metal substrates for surface-enhanced Raman scattering

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Raman spectroscopy has long been regarded as a tool for the identification of chemical and biological molecules. However, very small cross-sections of Raman scattering have limited its applications in many fields. Surface-enhanced Raman scattering effect, which results from the adsorption of molecules on plasmonic metal surfaces, is one of the remarkable ways to enhance the efficiency of the Raman process.In this work, we have synthesized various gold and silver metal nanoparticles or surfaces in different sizes and shapes and have tested the sensitivity for surface-enhanced Raman scattering. We have measured and analyzed Raman spectra of amino acids including glycine and alanine adsorbed on these metal nanoparticles or surfaces.

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Synthesis, Characterization of PEI-FITC Coated Gadolinium Oxide Nanoparticles as a Dual Imaging Contrast Agent

Xu Wenlong Badrul Alam Bony tirusew tegafaw 김성준 Md. Wasi Ahmad MiaoXu 이강호*

경북대학교 화학과

We report PEI-FITC surface modified gadolinium oxide nanoparticles in phosphate buffer solution. We found that nanoparticles are monodisperse with ~2 nm diameter. They were characterized with XRD, FT-IR, Fluorescence spectrophotometer, TGA, SQUID magnetometer, TEM and MRI instrument. These nanoparticles have fluorescence at ~ 524 nm and enhanced relaxivity. Hence, it can be used as a dual MR-FL imaging contrast agent.

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Vacuum ultraviolet mass-analyzed threshold ionization spectroscopy (VUV-MATI) of cyanopyrazine

강도원 김홍래* 권찬호*

강원대학교 화학과

We applied the vacuum ultraviolet mass-analyzed threshold ionization (VUV-MATI) technique to record the vibrational spectrum of cyanopyrazine cation in electronic ground state and for the first time, obtained the vibrational spectrum in the VUV photon energy range of 80220-81320 cm^{-1}. Twelve vibrational peaks in the VUV-MATI spectrum were observed and assigned by utilizing vibrational frequencies and Franck-Condon factors calculated at B3LYP level with the cc-pVTZ basis set. The structure of cyanopyrazine cation in electronic ground state was determined, based on good agreement between the experimental and calculation results. In addition, the adiabatic ionization energy of cyanopyrazine was determined to be 9.9582 ± 0.0009 eV (80318 cm^{-1} ± 7 cm^{-1}).

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Photodissociation dynamics and potential energy surface of acetic acid at 205 nm

박성만 권찬호 김홍래*

강원대학교 화학과

Photodissociation dynamics of H atom production channels from acetic acid at 205 nm has been investigated by measuring translational energies of the H atom products. The spectrum of H atom was measured by laser-induced fluorescence from the 3s, 3d to the 2p state (Balmer-α line) induced by two photon absorption from the 1s state. From Doppler profile analysis in the spectra, translational energy releases are determined for H atom dissociation channels of CH_2COOD + H and CH_3COO + D.Quantum chemical calculations have been performed to construct potential energy surfaces for the ground and electronically excited states leading to the individual product channels and the spin correlation suggests that dissociation of acetic acids producing the H atoms should take place on the triplet state

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Excited-state dynamics of carotenoids between the S2 and S1 electronic states

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광주과학기술원(GIST) 물리화학부

Carotenoids are natural pigments in plants and photosynthetic bacteria which play important roles in photosynthesis such as light-harvesting and photoprotection. Carotenoids absorb a blue-green region of sunlight in which chlorophylls do not have absorption, and transfer to chlorophylls. They also protect the reaction center complexes from excess energy by quenching the singlet or triplet excited states of chlorophylls. Carotenoids have been studied by time-resolved laser spectroscopy ot unveil the efficient energy transfers which might be related to their ultrafast excited-state dynamics in the singlet states. In this study, 8'-apo-β-caroten-8'-al dissolved in chloroform and n-hexane have been investigated by femtosecond transient absorption spectroscopy. Pump pulses at 480 nm are used to excite molecules into the lowest vibronic level of the S2 state and three temporal components including the well-known lifetimes of the S2 and S1 states have been found in the kinetic analysis of transient absorption spectra. Additional ultrafast temporal component in the excited-state dynamics of 8'-apo-β-caroten-8'-al might provide keys to solve the exceedingly complex dynamics of carotenoid between the S2 and S1 states, which might be originated from a dark S* state or the S1/ICT state.

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BSA Conjugated Gd_2O_3 Nanoparticles as a MRI Contrast Agents

Md. Wasi Ahmad **Xu Wenlong Badrul Alam Bony tirusew tegafaw 김성준 MiaoXu 이강호**[*]

경북대학교 화학과

Bovine serum albumin (BSA) (Mn = 66.5 kD, size = 14 x 4 x 4 nm) as a carrier molecule of various ions and molecules in blood plasma is an attractive biological molecule for biomedical applications in nanomedicine because it can carry ultrasmall nanoparticles (NPs) owing to its large size and mass. Thermogravimetric analysis showed that BSA could bind ~ 9 surface modified Gd_2O_3 NPs (GNPs) (d_{avg} = 2.0 nm) with polyethylene glycol diacid (PEGD) through amide bonding. High relaxivities ($r_1 = 6.0\ s^{-1}mM^{-1}$ and $r_2 = 28.0\ s^{-1}mM^{-1}$) were observed in an aqueous sample solution. During 3 tesla T_2 magnetic resonance imaging (MRI) of a mouse, the injection of an aqueous sample solution into its tail vein revealed significant negative contrast enhancements. On the other hand, cleaved BSAs (C-BSAs) (Mn < 7 kD) could bind only ~ 0.2 surface modified GNPs with PEGD because of their reduced size and mass that were similar to polymers.

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Theoretical Studies for Multiple Proton Transfer in Calix[4]arene derivatives

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Calixarene 은 모방효소, ion sensitive 전극이나 센서에서 적용될 뿐만 아니라 나노기술에서 고해상도 전자빔 리소그래피의 negative resist 로써 사용되는 화합물이다. 본 연구에서는 calix[4]arene 과 tert-p-nitro calix[4]arene 의 tetrachloroethene 용액내에서 내부 양성자 이동을 알아보았다. 반응물과 전이상태, 생성물의 최적화 구조를 M06 계열의 M06-2X DFT 방법과 6-311+G(d,p), STO-3G 의 두 가지 basis set 를 혼합하여 계산하였다. 다차원 터널링 근사 및 변분법적 전이상태이론으로 반응동역학 계산으로부터 반응속도를 구하고 반응속도론적 동위원소 효과를 확인하였다.

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Dockable Pocket Site Prediction (DPSP) for annotation of protein function

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Protein binding pocket is essential for signal transduction and reactant generation in vivo, so information of ligand and protein binding site position is important for understanding mechanisms. However, most of protein-ligand binding site and interaction details are unknown. Here, DPSP, a method to find protein binding site using geometry method and annotate ligand information based on protein only structure database. DPSP finds match protein sequence in database which has 84,600 structures and ligand information is gathered. After finding matched protein structures, DPSP chooses binding site which has high Matthews correlation coefficient and implements ligand docking process for more specific ligand position. DPSP was tested on 10 proteins which are CASP10 FN targets. In CASP10, we got a Matthews correlation coefficient about 0.27 among 10 targets. The top three scores have over 0.6 (30%). When we applied docking system, Matthews correlation coefficients were 0.25 (the lowest energy dose) and 0.49 (the best docking dose). This method is expected to use drug research efficiently in the way that it predicts binding site and ligand information of unknown protein binding mechanisms. Also, by providing various ligand candidates, it will help a researcher to select the ligand in researcher’s case.

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NmRe : NMR protein structure refinement web server

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The structure refinement is necessary step for research of protein structure function. In particular, some nuclear magnetic resonance (NMR) structures have a lower quality than X-ray crystallography structures. The NmRe web server provides a NMR protein structure refinement. The default refinement is performed with target energy potentials developed by our group: STAP (Statistical Torsion Angle Potential) and structural-derived distance potential. The STAP is two-dimensional Ramachandran potential based on torsion angle combinations of backbone and side-chain. The structural-derived distance potential is made by distance information from the given structure in order to prevent a structure to largely deviate from the original structure during a refinement process. The NmRe refinement efficiency was validated on 20 NMR structures and refinement targets from CASP8, 9, and 10. The most of quality assessment scores of NMR structures showed better quality than their original structures (normalized quality score increased from 1.06 to 1.89). CASP targets were slightly improved (from 1.94 to 2.03 (CASP10) and from 2.22 to 2.40 (CASP8)). The results of refinement are provided by 3D structure and secondary structure scheme and tabulated by various quality assessment scores.

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Photo-enhanced D band of oxidized graphene on SiO_2/Si substrates

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그래핀(graphene)은 sp^2 혼성화를 이루는 단결정 물질로서 열에 대한 높은 안정성과 뛰어난 전기적 특성을 가지고 있다. 구조적 결함은 그래핀의 물성을 변화시키기 때문에 이러한 결함을 제어하고 분석하는 것은 중요한 일이다. 고온 산화처리를 통해 그래핀의 결함을 증가시키면 라만분광법을 통해 D-피크를 관찰할 수 있다. 본 연구에서는 AFM(원자힘현미경)을 이용하여 고온에서 산화처리된 그래핀에 나노공(nanopore)이 생성되었음을 확인한 후, 라만 분광법을 이용하여 D-피크의 변화를 관찰하였다. D-피크의 크기는 레이저의 세기와 노출 시간에 따라 증가되는 것을 관측하였다. 이러한 D-피크의 증가는 기존에 연구되었던 산화처리된 그래핀에서 나타나는 D-피크의 생성과는 다른 경향을 보이며, 산화 열처리 과정에 의해 생성된 변화가 그래핀의 열에 대한 안정성을 감소시켰다고 예상된다.

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Raman spectroscopy study of single and few-layer MoS_2

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그래핀(graphene)의 연구가 활발히 진행됨에 따라 유사한 2 차원 물질인 MoS_2 도 함께 차세대 물질로서 각광을 받고 있다. MoS_2 의 두께에 따른 E^1_{2g}(in-plane mode), A_{1g}(out-of-plane mode) 피크의 진동수 변화는 잘 알려져 있으나, E_{1g} 피크에 대한 연구는 아직 미진한 실정이다. 본 연구에서는 MoS_2 시료에서 열에 의해 유발되는 결함의 영향, 산소 플라즈마 반응에 의한 영향, 그리고 입사광의 편광에 따른 E_{1g} 피크의 변화를 살펴보고자 한다. 기계적 박리법을 이용하여 MoS_2 결정으로부터 단일층 및 복층의 MoS_2 를 분리하여 SiO_2/Si 기판에 전사한 후 상기한 대조군에서 E_{1g} 진동모드의 특성을 관찰하였다.

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Vibrational frequency shifts - fully first principles theory for simple vibrational chromophores

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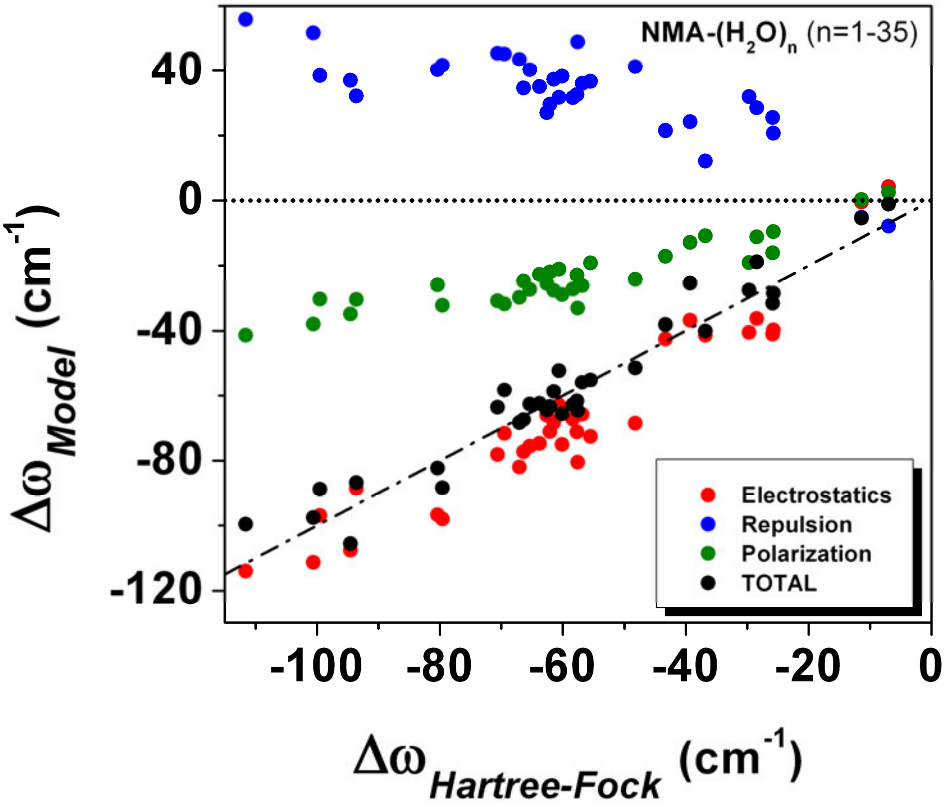
Vibrational infrared (IR) frequency shift is directly related to the solute-solvent interaction-induced effects in condensed phases. Experimental studies of frequency shifts of small vibrational probes can be useful in understanding the dynamics and probing the local molecular environments.[1] However, proper interpretation of IR experimental data requires accurate theoretical model. The great majority of proposed approaches is based on semi-empirical procedures employing various fitting to benchmark ab initio calculations or experimental data.In this presentation we outline the fully first-principles theory of vibrational solvatochromism which is based on coarse-grained models developed by Cho.[2] The solvation-dependent observable is described in these models as a function of gas-phase properties of solute and solvent molecules. We have already shown that taking into account electrostatic interaction only one can quantitatively predict frequency shifts of N-methylacetamide (NMA) amide I mode in small NMA-(H2O)n (n=1-35) complexes.[3] Recently, we have extended our theory and included also exchange-repulsion, polarization and charge-transfer interactions. By using the presented model it is possible to study very large systems.References[1] H. Kim, M. Cho, Chem. Rev. 113 (2013) 5817-5847[2] M. Cho, J. Chem. Phys. 130 (2009) 094505[3] B. Błasiak, H. Lee, M. Cho, J. Chem. Phys. 139 (2013) 044111


NMA-$(H_2O)_n$ (n=1-35)
Electrostatics
Repulsion
Polarization
TOTAL
40
0
-40
-80
-120
-100
-80
-60
-40
-20
0
$\Delta\omega_{Model}$ (cm^{-1})
$\Delta\omega_{Hartree\text{-}Fock}$ (cm^{-1})

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Synthesis of Magnetite (Fe3O4) Nanoparticles Coated with Mesporous Silica (SiO2)

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In the present work we present the synthesis of magnetite nanoparticles with different sizes, maintaining their structure and composition to the unique phase. Employing hydrothermal method with varied synthesis parameters, the size and morphology of the nanoparticles could be controlled. Using hydrated ferrous and ferric chlorides in acidic aqueous medium, we could generate magnetite nanoparticles of about 29 nm average size. On the other hand, using only one iron precursor (FeCl3?6H2O) in ethylene glycol solution, we could obtain magnetite nanoparticles of 208 nm average size. Both kinds of particles were coating with mesoporous silica through the modified St?ber method.

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The Comparison of Adsorption Structures of 2-Mercaptoethanol and Thioglycolic acid on the Ge(100) Surface

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The adsorption selectivities between 2-mercaptoethanol (ME) and thioglycolic acid (TGA) were revealed through density functional theory (DFT) calculations of the respective stable adsorption structures, transition state energy, and reaction pathways when they adsorbed on the Ge(100)-2x1 surface. The DFT calculations suggested that most stable and reasonable pathway to adsorb ME and TGA on the Ge(100) surface, respectively. Moreover, in order to identify the most probable adsorption structures with their electronic properties of two molecules on Ge(100) surface, we have conducted experiment by HRPES to obtain adsorption structure data depending on coverages. HRPES analysis corroborated by DFT calculations, indicated that O dative bonded structure of ME at high coverage and O-H dissociated S-H dissociation bonded structure at low coverage are stable structures on Ge(100) surface. In addition, S-dative bonded structure of TGA at high coverage and S-H dissociated O2 dative bonded structure at low coverage are reasonable adsorption structure on Ge(100) surface.

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Computational Studies on Thermal Degradation of PET, PTT and PBT

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Studies on the thermochemistry and kinetics of the thermolysis of PET (poly(ethylene terephthalte)), PTT (poly(trimethylene terephthalte)) and PBT (poly(butylene terephthalte)) have been conducted using density functional theory (DFT). Despite of structural similarities, it has been reported that those three polymers show quite different behaviors in thermal degradation at least as far as the final products are concerned; i.e., thermal degradation of PET produces the anhydride-containing oligomers while PTT and PBT the alkenyl-ester terminated ones. Calculations on the ground state of reactants and products have been carried out using B3LYP/6-31G(d,p) method, and the transition structures were calculated by the STQN method with the QST2 and QST3 options. The rate constants for the main steps involved in the thermal decomposition of PET, PTT and PBT have also been calculated using the transition state theory (TST). From the constructed potential energy diagrams and kinetic simulations, plausible reaction pathways for the thermal degradation of poly(alkylene terephthalate) have been suggested to explain the experimentally determined reaction products.

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The Improvement of Kinetic Theory of Ideal Gases and the Development of Kinetic Theory of a Particle Solution, based on Discovering the Maximum Net Energies of the Particles and the Solvent Molecules Available for Their Useful Works

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There are two correct thermodynamic equations. One is that, in the case of the earth atmospheric equilibrium system in which ideal gas mixture of binary components i and j are in the gravitational equilibrium, according to Gibbs thermodynamic theory, the two conditions given by $\mathrm{d}\mu_{IGi} = RT\mathrm{dln}P_j = M_i g\mathrm{d}h$ and $\mathrm{d}\mu_{IGj} = RT\mathrm{dln}P_j = M_j g\mathrm{d}h$ (called the Gibbs equations) are necessary and sufficient for constructing the atmospheric system, where μ is the free energy of the ideal gas at an altitude of h; the subscription "i" (or "j") stand for the gaseous component. Where P, R and T have their usual meaning, g the acceleration of gravity; M_i and M_j are the molecular weights of component i and j. The other is that in the case of the true gravitational system consisting of an inhomogeneous particle solution of different size molecules and different activities, we have Guggenheim's thermodynamic equation given by $N_p\mathrm{d}\mu_p + N_s\mathrm{d}\mu_s = - N_pV^*_p(D_p - D)g\mathrm{d}h - N_sV^*_s(D_s - D)g\mathrm{d}h = 0$ obtained from Gibbs-Duhem relation. This equation informs that the true free energies, μ_p and μ_s, considered by Guggenheim, balancing the true net gravitational potential are, respectively, $\mathrm{d}\mu_p = - N_sV^*_sM_pg\mathrm{d}h + N_sV^*_pM_sg\mathrm{d}h$ and $\mathrm{d}\mu_s = - N_pV^*_pM_sg\mathrm{d}h - N_pV^*_sM_pg\mathrm{d}h$ (called the Guggenheim's equations). In the case of real solution of same-size molecules, we have $\mathrm{d}\mu_p = RT\mathrm{dln}a_p$ and $\mathrm{d}\mu_s = RT\mathrm{dln}a_s$ both are adapted in modern thermodynamic theory of solution that hold in the real solutions of different activities and, in fact, in same-size molecules. Comparing between the Gibbs equations and those Guggenheim's equations informs that the unique state equations for true free energies that satisfy both the true gravitational equilibrium and the Gibbs-Duhem relation must be obtained by replacing the factors, $M_pg\mathrm{d}h$ and $M_sg\mathrm{d}h$, in the Guggenheim's equations with those adopted equations for $\mathrm{d}\mu_\mathrm{p}$ and $\mathrm{d}\mu$ as $\mathrm{d}\mu_{Gu,p} = - N_sV^*_sRT\mathrm{dln}a_p + N_sV^*_pRT\mathrm{dln}a_s$ and $\mathrm{d}\mu_{Gu,s} = - N_pV^*_pRT\mathrm{dln}a_s +$

$N_pV^*_sRT\text{dln}a_p$. Using these unique state equations and adopting the equipartition principle, the following (a) to (h) are successfully illuminated through basic dynamic mechanical methods, and the correctness of these state equations are judged from these successes. Using the mechanical lever rule (a) the Raoul's law and (b) van't Hoff's law are derived; (c) the equation is directly reduced to $d\mu_p = RT\text{dln}X_p$ and $d\mu_s = RT\text{dln}X_s$ in the case of ideally dilute particle solution, where X_p and X_s are the mole fractions of components p and s; (d) Einstein's solute bombardment theory is proved to be correct; (e) an unified theory for the mechanism of osmotic equilibrium that harmonize perfectly with the law of action reaction, and (f) mechanical structure of Perrin's atmospheric equilibrium that harmonize perfectly the Newton's third law are presented.

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Bandgap of $AgInS_2$ Ⅰ-Ⅲ-Ⅵ semiconductor quantum dot

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Semiconductor quantum dots (QDs) have potential for application to electronic device, light emitting diodes (LED), solar cell, and photocatalysis because of their unique electronic and optical properties. II-VI Semiconductor QDs are well developed for these applications. However, II-VI semiconductor QDs include toxic heavy metals such as Cd, Pb, Hg, Se. Therefore, semiconductor QDs with nontoxic element are required. In this regard I-III-VI type semiconductor QDs such as $CuInS_2$, $AgInS_2$, and $AgGaS_2$ have been studied for alternatives of II-VI semiconductor QDs. When we studied the defect emission of $AgInS_2$ QDs, we observed unexpected emission around 500 nm reproducibly. So we investigated the origin of this emission. In time-integrated photoluminescence (TIPL) spectra, the emission around 500 nm was deconvoluted by two species (480 nm, 509 nm), which are explained by crystal-field splitting. And we found that these species have different lifetimes. The time decay profiles of the emission were fitted by triexponential model. These liftetimes were distinguished from those of the defect emission. Therefore we suggested that the emission around 500 nm is the bandgap emission of AgInS2.

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Revealing the Origin of Quantum Coherence in Chlorosome using Two-Dimensional Electronic Spectroscopy

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Chlorosomes, the most efficient photosynthetic light-harvesting complexes found in nature, consist of many bacteriochlorophyll (BChl) molecules self-assembled into supramolecular aggregates. In this work, we elucidate the dynamics of ultrafast downhill energy transfer and the origin of coherent oscillations in chlorosome isolated from Chlorobaculum limnaeum at cryogenic temperature using two-dimensional (2D) electronic spectroscopy. The line shape of a major peak in 2D spectra changes rapidly on 20 ~ 30 fs time scale, and the line shape dynamics are attributed to ultrafast downhill energy transfer in coherent domains within a BChl layer in chlorosome. In addition, coherent oscillations superimposed on the ultrafast amplitude decay were observed distinctly, and we elucidated the origins of the oscillations from their Fourier analysis. In particular, the most pronounced oscillation of 140 cm^{-1} frequency was identified to originate from vibrational coherence, while the smaller oscillation of 620 cm^{-1} frequency arises from electronic coherence. Despite rapid dephasing of the coherent oscillation, the electronic coherence may still take part in the initial step of energy transfer, which is comparably fast, in chlorosome.

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Snapshots of Cytochrome c Folding Tracked by Time-resolved X-ray Solution Scattering

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Understanding the protein folding pathway with the characterization of intermediate structure is of importance in the fields of biochemistry and biophysics. Among many proteins, cytochrome c (Cytc), which is an essential component of electron transport chain in mitochondria, is an ideal model to investigate the global scheme of protein folding due to the structural simplicity. Although the extensive experimental and theoretical studies for the Cytc folding have been performed, it is hard to establish the folding framework of cytochrome c in view of the conformational change of protein owing to the lack of experimental probe that is sensitive to the global structural change. To overcome this, we employ pump-probe X-ray solution scattering to probe the folding pathway of Cytc induced by the electron transport reagent occurring in a wide time range from 31.6 μs to 316 ms. From the systematic analysis, the folding pathway of cytochrome c shows the two-state kinetic model (unfolded form → folded form) accompanying 117 ms as the rate constant. In addition, the hidden folding pathway, which is not detected in view of the global structural change, is captured by the thermodynamic analysis based on the heating response of solvent. From this study, we can unravel the folding dynamics of Cytc with the global structure of intermediate. The calorimetric analysis about the thermodynamics of solvent gives the kinetic evidence of the hidden folding pathway on the Cytc folding.

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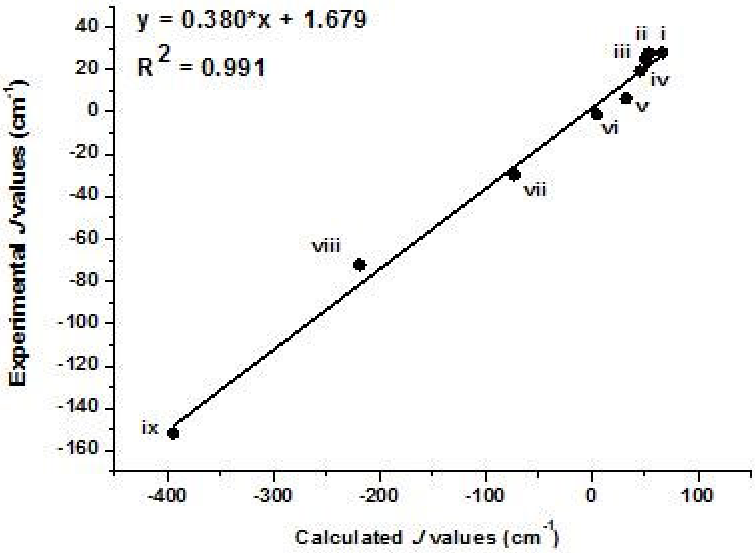
Scaling approach for Intramolecular Magnetic Coupling Constants for Stable Organic Diradicals Coupled with an Aromatic Ring: A DFT Study

조대흠 박영근 Kang baotao 문종훈 김선경 SHIHU 이진용*

성균관대학교 화학과

The intramolecular magnetic coupling constant (*J*) of 9 diradicals (i-ix) coupled with an aromatic ring were investigated by means of unrestricted density functional theory (DFT) calculations [B3LYP/6-311++G(d,p)]. For those diradicals, the linear correlation was found between the calculated and experimental *J* values on the basis of results of the linear regression analysis. In this study, we suggest that the value of slope (0.380) of linear regression can be used as scaling factor for estimating the accurate *J* values. In fact, DFT calculations overestimate the *J* values significantly. By applying this scaling factor to the calculated *J* values, we can predict the reliable *J* values of four DTDA diradicals (x-xiii) coupled with an aromatic ring. It also found that certain scaling factors have a restricted application depending on the length of a coupler unit. In conclusion, this approach, which uses a scaling factor, can be used to estimate the accurate *J* values for diverse diradical systems coupled with a particular coupler using DFT calculations.

Figure 1. Correlation between calculated and experimental *J* values (cm^{-1}) for 9 diradicals (i-ix) coupled with an aromatic ring.


y = 0.380*x + 1.679
R^2 = 0.991
i
ii
iii
iv
v
vi
vii
viii
ix
Experimental J values (cm^{-1})
Calculated J values (cm^{-1})
40
20
0
-20
-40
-60
-80
-100
-120
-140
-160
-400
-300
-200
-100
0
100

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Site-directed thermodynamic analysis on protein hydrophobicity

조한울 정성호 함시현*

숙명여자대학교 화학과

Hydrophobicity of a protein is considered to be a major factor controlling protein aggregation propensity, and its molecular understanding is of crucial importance in preventing protein aggregation diseases and in developing aggregation-resistant biotherapeutics. Usually, protein hydrophobicity is estimated as a sum of hydrophobicity scales for constituent amino acids, assuming that the hydrophobicity scales determined for individual free amino acids are not altered when amino acids are embedded in a protein. Here we investigate how the hydrophobicity of amino acids depends on the protein context by computing the solvation free energy of a protein and by decomposing it into contributions from constituent amino acids.

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Kinetic studies of solvolytic reactions of alkyl chlorothioformates using extended forms of the Grunwald-Winstein equation

박경호 경진범*

한양대학교 과학기술대학 응용화학과

The solvolysis rates of alkyl chlorothioformates (methyl-, ethyl-, *n*-propyl-, *i*-propyl-, *t*-butyl, 1-adamatyl- and 2-adamantyl-) are studied in pure and binary solvent mixtures. The linear free energy relationship and the sensitivities to changes in solvent nucleophilicity and solvent ionizing power of the solvolytic reactions are analyzed using the Grunwald-Winstein equation. The kinetic solvent isotope effects and the activation parameter values for the solvolyses of both substrates are also determined in additional. These observations are compared with those previously reported for the corresponding alkyl chloroformates and fluoroformates.

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The *ortho*-Substituent Effect of 2-(Trifluoromethoxy)benzoyl Chloride in Solvolysis

박경호 경진범* **Dennis N. Kevill**[1]

한양대학교 과학기술대학 응용화학과 [1]Northern Illinois University, U. S. A.

The solvolysis of 2-(trifluoromethoxy)benzoyl chloride was studied in usual reaction conditions, 25.0 ^{o}C, pure and binary solvents with water, and the conductivity method. Rate constants were analyzed by simple and extended Grunwald-Winstein equations and compared with previously reported other benzoyl chlorides for confirming the reaction mechanism. The solvolysis of 2-(trifluoromethoxy)benzoyl chloride was showed different aspect compared with previously reported 2-methoxy and 2-chloro derivatives, because *ortho*-substituent, 2-trifluoromethoxy group, has electron withdrawal effect and large steric hindrance at reaction center, carbony carbon, so dual pathways were observed with several evidences, kinetic solvent isotope effect and thermodynamic parameters.

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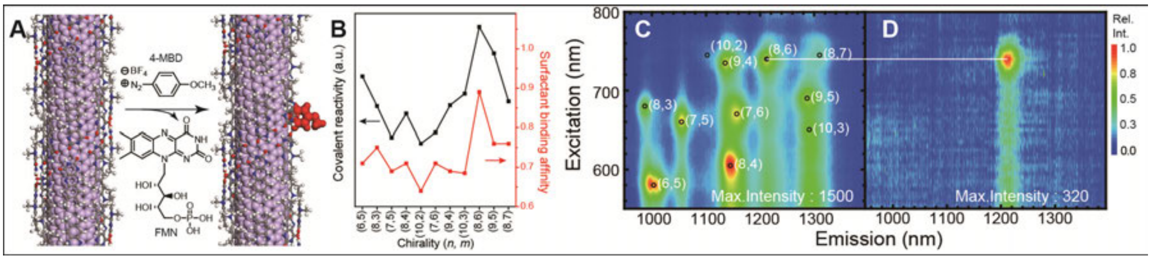
Specific Chirality Separation of Carbon Nanotubes by Controlling Surface Reactivity via Flavin Mononucleotide

심진숙 장명수 주상용*

연세대학교 화학과

Defined electronic types of single-walled carbon nanotubes (SWNTs) are essential to realize nanotube as high-performance field effect transistors as well as other sensor applications. While tremendous advances have been made in selectively reacting metallic nanotubes and semiconductor nanotubes according to diameter, but the underlying role of surfactant organization is poorly understood. We show that nanotube reactivity after covalent diazonium modification is governed by a chirality-specific surfactant binding affinity to SWNTs. Unlike sodium dodecyl sulfate (SDS) displaying SWNT diameter-dependent reactivity, tight wrapping of flavin mononucleotide (FMNs) on SWNTs resulted in resistance of the SWNTs to chemical functionalization with diazonium reagent, and these SWNTs exhibited distinctive reactivity kinetics and energy transfer patterns according to nanotube chirality and electronic type. These specific behaviors are confirmed by absorption, Raman, and PL spectroscopy. Irrespective of electronic type, this nanotube reactivity was similar to that of FMN wrapping stability on carbon nanotubes, as probed by binding affinity assessments using noncovalent surfactant exchange. Reactivity of both metallic and semiconducting SWNTs originates from binding affinity of FMN to carbon nanotubes, showing metallic tubes marginally preferred reactivity. With information of this selective reactivity, single chirality enrichment of SWNT is demonstrated. These findings provide insight into the chemical reactivity of nanotubes and indicate that it may be possible to achieve specific chiralities using surfactant-SWNT binding affinity.Figure 1. (A) Schematic illustration of the reaction of 4-MBD on FMN-wrapped SWNTs, (B) showing similar degree of chirality-dependent covalent reactivity with diazonium salt and FMN binding affinity, PLE maps of (C) before and (D) after 45h reaction of 0.3mM 4-MBD with FMN-SWNTs.


A
4-MBD
⊖BF4
⊕N2
OCH3
FMN
HO
OH
HO
OH
O
P
OH
NH
B
Covalent reactivity (a.u.)
Surfactant binding affinity
0.6
0.7
0.8
0.9
1.0
(6,5)
(8,3)
(7,5)
(8,4)
(10,2)
(7,6)
(9,4)
(10,3)
(8,6)
(9,5)
(8,7)
Chirality (n, m)
C
D
800
700
600
Excitation (nm)
(10,2)
(9,4)
(8,6)
(8,7)
(8,3)
(7,5)
(7,6)
(9,5)
(10,3)
(8,4)
(6,5)
Max.Intensity : 1500
Max.Intensity : 320
1000
1100
1200
1300
Emission (nm)
Rel. Int.
1.0
0.8
0.5
0.3
0.0

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Enhanced performance of CdS/CdTe quantum dot-sensitized solar cells containing single-walled carbon nanotudes

신호경 이종택 이휘건*

한양대학교 화학과

We fabricated quantum dot-sensitized solar cells using CdS and CdTe quantum dots (QDs) as sensitizers. CdS QDs were deposited on spin-coated TiO_2 layer by a successive ionic layer adsorption and reaction method. Pre-synthesized CdTe QDs were adsorbed on CdS QDs layer using a direct adsorption technique. A QD-modified working electrode and a Au counter electrode were assembled as a sandwich type cell and polysulfide electrolyte solution was inserted between the working electrode and the counter electrode. Single-walled carbon nanotubes (SWNTs) were incorporated in our cells as p-type semiconducting materials due to their efficient hole-transfer capability. The SWNTs were mixed with TiO_2 paste or were sprayed between layers. The effect of SWNTs in our cells was analyzed by solar simulator and electrochemical impedance spectroscopy. The performance of cells containing SWNTs was mostly enhanced. Specifically, the cell using TiO_2 paste mixed with SWNTs exhibited a 24% increase in photo-current conversion efficiency.

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Enhancement of ZnO nanowire with photo-current conversion efficiency in CdS/CdSe quantum-dots solar cell

이준영 박태희 이휘건*

한양대학교 화학과

Zinc Oxide (ZnO) nanowire is known as a material has good charge carrier mobility, Nanowire structure also have advantage of short travel range and direct pathway of charge carrier than porous shape so that it can provide efficient charge carrier transfer in photovoltaic devices. ZnO nanowire fabricated on Fluorine-doped tin oxide (FTO) glass. ZnO sputtering seed layer deposition on FTO and then dipping $Zn(NO_3)_2$ and Hexamethylentetramin(HMT) solution. We confirm X-ray diffraction (XRD) ZnO crystalline. Cadmium sulfide (CdS) and Cadmium selenide (CdSe) quantum dots were deposited on ZnO nanowire successive ionic layer liquid adsorption and reaction (SILAR) method. We used solar simulator that measurement solar cell illuminate 100mW/cm2 , AM1.5. The results show that CdS and CdSe QDs have a complementary effect in the light harvest and the performance of QDs solar cell.

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Infrared absorption spectra of Iron Dinitrogen Complexes isolated in solid Ne

고은미* **조수경[1]** **배광태[2]**

국방과학연구소 국방신기술본부 국방고등기술원 [1]국방과학연구소 국방고등기술원 [2]국방과학연구소 국방고등기술원/첨단기술 연구센터

Iron Dinitrogen Complexs generated during Laser-ablation and Matrix isolation system $Fe(NN)_x$ were analyzed via FTIR. The FTIR spectra show the formation of series of complexes, and comparison with theoretical predictions from density functional theory calculations.

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Dissociation and Association Dynamics of Potassium Thiocyanate in solution: A QM/MM-MD Study

남혜림 **Manik Kumer Ghosh** 최철호*

경북대학교 화학과

I will discuss about association/dissociation of Potassium thiocyanate simulated by QM/MM-MD method. Umbrella sampling was performed to get free energy corresponded to the ion association. We will see the structure of Potassium thiocyanate and how some water molecules make bridge with it when the potential of mean force has minimum. Interesting fact is that potassium ion prefers nitrogen side more than sulfur side of thiocyanate when free energy is most stable. Indeed by the radial distribution function, water molecules have more interaction with Sulfur than nitrogen. So now we can guess because of water molecule's interruption, potassium ion should be located in nitrogen side relatively. This phenomenon appears in the same way in quantum mechanics simulation.

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Band structures and optical properties of noble metals and their alloys: a theoretical study

김진영 류설*

조선대학교 화학과

We calculate the electronic band structures of both pure noble metals and their binary-component alloys, using density functional theory methods with plane-wave basis sets. We will investigate how the different components modify the band structures, density of electronic states, and permittivities. As the mixed-component metal or alloy-like nanoparticles have recently been synthesized, the necessity of having reliable permittivity values for such metal systems may increase for theoretical simulations. It is noteworthy that correct permittivity values for mixed metal systems are not necessarily simple linear combinations of individual components' which were usually experimentally collected and also that the experimental values may be limited in practical use for mixed metal systems. This study may allow us to assess the feasibility of fine-tuning the optical properties of metal nanoparticles via intrinsic permittivity controls.

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DFT study of phosphorescent heteroleptic Ir(Ⅲ) compounds

이지혜 송연호 황현석*

강원대학교 화학과

The electronic and optical properties of heteroleptic Ir(Ⅲ) compounds are investigated using the density functional theory. The optimized geometries and isodensity surfaces of the HOMO and the LUMO for heteroleptic Ir(Ⅲ) compounds at the S_0 and T_1 were performed at the B3LYP and PBE0. The LANL2DZ is used for the Ir and the two basis sets (6-31G(d) and 6-31+G(d)) for all the other atoms in the calculation. From this calculations, $S_0 \rightarrow T_1$ adiabatic energies (△SCF) were obtained. Also, $S_0 \rightarrow T_1$ vertical excitation energies were performed by TD-DFT calculations at the same level for the ground states. Natural transition orbitals (NTOs) were also calculated. The results for the heteroleptic Ir(Ⅲ) compounds obtained from this study were compared with experimental results. Through the comparison, several issues are discussed.

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Energetics and dynamics of β-D-glucose transport through a cyclic peptide nanotube: A molecular dynamics study

서용일 황현석*

강원대학교 화학과

Cyclic peptide nanotubes (CPNs) which assume tubular hollow structures like natural ion channels can transport alkali metal ions through themselves. CPNs also transport small bio molecules such as β-D-glucose. It is of great importance to understand energetics and dynamics of the transport of small bio molecules through CPNs in terms of drug delivery. In this study, we perform molecular dynamics (MD) simulations of the transport of β-D-glucose through a CPN composed of 8 × [-(D-Leu-L-Trp-)$_4$-D-Leu-L-Gln-] embedded in 1,2-dimyristoyl-sn-glycero-3-phosphocholine (DMPC) lipid bilayers. For the study of energetics of the β-D-glucose transport, potential of mean force (PMF) profiles are calculated using the umbrella sampling (US) as well as the thermodynamic integration (TI) method. Dynamical behaviors of the β-D-glucose transport are elucidated by calculating the position-dependent diffusion coefficients of β-D-glucose inside the CPN.

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The effect of lipid bilayer hydration of energetics of K^+ ion transport through a cyclic peptide nanotube: A molecular dynamics study

송연호 황현석*

강원대학교 화학과

Cyclic peptide nanotubes (CPNs) are synthetic tubular proteins which allow ions and small molecules to permeate through lipid bilayers. In this study, we perform molecular dynamics (MD) simulations to investigate the influence of lipid bilayers hydration on the energetics of ion transport through CPNs. To this end, we calculate potential of mean forces (PMFs) of a K^+ ion through a CPN in hydrated 1,2-dimyristoyl-*sn*-glycero-3-phosphocholine(DMPC) lipid bilayers via the umbrella sampling (US) and adaptive biasing force (ABF) methods. To examine the dependence of the PMF profiles on the fluctuation of lipid bilayer hydration, steered molecular dynamics (SMD) simulations are also conducted. The results reveal that interactions between headgroups (ester group, PO_4 and $N(CH_3)_3$) in DMPC lipids and a K^+ ion have considerable effects on the energetic of ion transport. The variation of the solvation shell around the K^+ ion also brings about the variation of energetics.

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페로센과 그 유도체의 이온화포텐셜계산에서 여러가지 밀도범함수의 성능평가

우동주 이상연*

경북대학교 응용화학과

전이금속화합물은 레독스흐름전지의 활물질로 사용하는 경우가 있다. 보다 성능이 우수한 활물질의 설계하기 위하여, 전이금속화합물의 산화환원쌍의 표준환원전위를 이용하기도 한다. 전이금속화합물의 표준환원전위를 계산을 위하여, 산화환원쌍의 이온화에너지와 용매화에너지의 차이가 필요하다. 이들 에너지들은 보통 밀도범함수계산결과를 얻을 수 있다. 계산결과의 정확성은 계산에 이용하는 밀도범함수와 기본조함수에 따라 다르다. 본 연구에서는 다양한 밀도범함수를 이용하여 페로센과 그 유도체의 이온화에너지를 계산하고, 계산된 이온화에너지들을 실험값과 비교하여, 전이금속화합물에 대한 밀도범함수의 성능을 평가하였다.

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The Solvation Dynamics of formamide by Quantum Mechanical Molecular Dynamics

<u>백용수</u> 최철호[*] Manik Kumer Ghosh

경북대학교 화학과

Peptide bond hydrolysis is a key biochemical reaction in both intracellular and extracellular regions. But the reaction mechanism for the neutral hydrolysis of amides in water has not been yet established. Though there is some experimental evidence that uncatalyzed hydrolysis occurs in water in neutral pH, the corresponding reaction mechanism is controversial. In this work, we have investigated in detail the possible mechanism of the hydrolysis of formamide in aqueous solution. A combined quantum chemical calculations and quantum mechanical molecular dynamic (QMMD) simulations have been performed though this work. A both concerted and step-wise reaction mechanism has been considered. An ab-initio quantum mechanical calculation further support the findings in QM/MM-MD simulations

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IR correlation spectroscopy to detect a target gas using its micrograting

최은우 조충만 김성규*

성균관대학교 화학과

Eunwoo Choi, Choong-Man Jo, Seong Kyu KimDepartment of Chemistry, Sungkyunkwan University, Suwon 440-746, KoreaUsing a gradient searching error minimization method, we designed the patterns of microgratings which can retrieve the IR spectra of several target gases. Especially, the designed microgratings for SF6 and NH3 were fabricated by a series of etching process using four masks on a silicon wafer in 19.2×19.2 mm2 size. Each micrograting has 1441 reflecting lines of 13.323 μm width, whose depths are discretized into 16 levels between 0 and 6.9 μm. When monitored at 15o angle, each micrograting generated the IR spectrum in good agreement with the reference one. The diffraction spectrum can be shifted linearly with diffraction angle, which provides a modulation necessary for the correlation spectroscopy. We demonstrate the correlation signal detected for SF6 or NH3 gas in nitrogen atmosphere. We also show cross-correlation simulations for numerous gases in the spectral range of 750 ? 1400 cm-1, which may provide criteria to identify the target gas from the correlation signal.

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Free radical initiated peptide sequencing (FRIPS) used for de novo sequencing

남정주 오한빈*

서강대학교 화학과

FRIPS (free-radical initiated peptide sequencing) approach is a recently developed peptide sequencing method that makes use of odd-electron radical-driven fragmentation chemistry. In this study, we incorporate the bromine atom in the N-terminal TEMPO-derived conjugated radical initiator, for example, at the ortho position of the benzyl group, in order to utilize the unique isotopic pattern of bromine for the purpose of distinguishing N-terminal fragments from C-terminal fragments. Indeed, the bromine-incorporated TEMPO-Bz- conjugated group gave rise to the unique isotopic pattern that facilitates the easy identification of N-terminal peptide fragments. We demonstrate in this study that by utilizing bromine of a unique isotopic pattern de novo sequencing of peptides can be easily accomplished without the aid of other fragment identification algorithm.

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Free radical initiated peptide sequencing (FRIPS) mass spectrometry spectra is simplified by guanidination of peptides

전애란 오한빈*

서강대학교 화학과

The TEMPO-based FRIPS method has been previously shown to be a powerful tandem mass spectrometry tool for peptide sequencing. However, in TEMPO-based FRIPS, a TEMPO-radical initiator can be attached to a lysine side chain as well as the desired N-terminus. It was often found that more than one initiator is attached to the peptides, which increases the complexity of the tandem mass spectrometry mass spectra. In order to facilitate the interpretation of FRIPS mass spectra, a lysine side chain is guanidinated, using the well-known guanidination protocol. With this method, it is assured that TEMPO-Bz-C(O)- conjugated group is attached to the desired N-terminus. Peptides prepared in this way were analyzed and it was found that the FRIPS tandem mass spectra is readily interpreted compared with those of putative peptides.

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장소: 일산KINTEX

발표코드: **ANAL.P-447**

발표분야: 분석화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Polyhexamethylene guanidine (PHMG) can be quantitatively analyzed using MALDI-TOF mass spectrometry

윤돈희 장인애 오한빈*

서강대학교 화학과

The long-term exposure to active ingredients of commercial disinfectants used in humidifiers was announced to be potentially involved in a large number of casualties related to pulmonary disease including at least four adult deaths. The active ingredients was identified as polyhexamethylene guanidine (PHMG). Recently, we have shown that qualitative analysis of PHMG oligomers can be made using MALDI-TOF mass spectrometry. In this study, we attempt for quantitative analysis of PHMG by applying the internal standard method. We have tested several internal standards which were chosen based on the structural similarity to PHMG; that is, the internal standards and PHMG contain a common structural motif of guanidine. Using this internal standard methods, the amount of PHMG could be determined over at least 5 orders-of-magnitude dynamic range with a modest reproducibility and linear response. Further experimental details will be shown in the symposium.

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Analysis of a tryptic peptide mixture using the free radical initiated peptide sequencing (FRIPS) nanoflow liquid chromatography-tandem mass spectrometry

장인애 오한빈*

서강대학교 화학과

Nanoflow liquid chromatography-tandem mass spectrometry (nano-LC-MS^n) was implemented to tryptic peptide mass spectrometry analysis using TEMPO-based free radical initiated peptide sequencing (FRIPS) approach. Tryptic peptides were conjugated with *o*-TEMPO-Bz-C(O)-NHS at the position of the N-terminus for TEMPO-based FRIPS application. The resulting *o*-TEMPO-Bz-C(O)-peptides were subjected to nano-LC-MS^3 analysis. Prior to analyze the tryptic peptide mixture, a model peptide mixture was successfully analyzed by nano-LC-MS^3. With this approach, it was possible to identify and characterize peptides under examination. With this combined approach, a few advantages could be achieved; for example, a less amount of samples and potential high-throughput analysis of complex peptide mixtures. In the symposium, further details of the experimental results will be discussed.

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발표코드: **ANAL.P-449**

발표분야: 분석화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

M13 박테리오파지 기반 신개념 세포 감지용 컬러 센서

이소영 김춘태 오진우[1,*]

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자연계의 많은 동식물들은 의사소통이나 분위기 표현, 위장 등을 하기위해 자신의 색을 바꾸는 것으로 알려져 있다. 현재 많은 연구자들이 이러한 자연 현상으로부터 영감을 받아 생체모방 구조와 메커니즘을 이용한 바이오센서를 개발하고 있다. 하지만 기존의 컬러센서는 수용체 개발에 있어 복잡한 디자인, 어려운 합성 방법 및 낮은 감도와 저선택성 등의 한계점을 가지고 있다. 이에 본 연구에서 우리는 바이러스(M13-박테리오파지)를 기반으로 한 신개념 고감도 고선택성 컬러센서를 개발하고자 한다. 우리가 개발하고자 하는 컬러센서는 자가 조립방법으로 만들어진 나노 구조체로 형성되어 있으며, 다양한 종류의 기체를 감지할 수 있다. 이 컬러센서는 아주 낮은 농도의 휘발성 유기화합물(volatile organic compounds)을 감지해 색변화를 보였으며, 다양한 독성 물질이나 방향족을 가진 화학 물질, 박테리아의 구분도 가능하였다. 따라서 우리가 개발한 컬러 센서는 임상 진단뿐만 아니라 식품 및 수질 컨트롤 등에 이용하여 국가의 안보나 국민의 건강을 증진시키기에 아주 유용할 것으로 보인다.

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

Detailed Chemical Characterization of Shale Oils Generated by Different Locations using Combination of Comprehensive 2D GC and Fourier Transform Ion Cyclotron Resonance Mass Spectrometer

조윤주 김성환*

경북대학교 화학과

It might be year or even decades before our energy and transportation infrastructure could be adapted to new energy sources despite the growing interest in using energy sources other than petroleum. Therefore, more research has to be done to develop unconventional hydrocarbon sources, like oil shale. Characterization of oil shale extracts is one of the important research fields that help utilizing the unconventional energy source. Therefore, wide range of analytical techniques including gas chromatography (GC) and Fourier transform ion cyclotron mass spectrometry (FT-ICR MS) has been used to characterize oil shale extracts. However, there has only a few studies applying combination of 2D GC and high-resolution mass spectrometry to compare the shale oils. In this study, saturates and aromatics fractions of shale oils generated by different locations were analyzed by using a thermal modulator connected to comprehensive 2D GC and atmospheric pressure photo ionization (APPI) FT-ICR MS was used to research Saturates/Aromatics/Resins/Asphaltenes (SARA) fractions extracted from shale oil at the molecular level. Anvil Points Mine (APM), Garden Gulch Member (GGM) and Uinta Basin Mahogany zone (UMZ) oil shale extracted by Fischer assay pyrolysis were used in this study. Each SARA fractions were compared between the data obtained by 2D GC and FT-ICR MS and it was shown that there was the difference between the locations of shale oils in terms of chemical compositions. Overall, we effectively combined two techniques, namely a positive-mode APPI FT-ICR MS and 2D GC-MS for more complete understanding of shale oils at low to high mass range ($50 < m/z < 1100$).

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

Effective Determination of NSAIDs in Aqueous Sample using Dispersive Liquid-Liquid Microextraction (DLLME) and HPLC-UV

박소연 명승운*

경기대학교 화학과

Dispersive liquid-liquid microextraction (DLLME) may be utilized as a green chemistry approach to reduce the consumption of hazardous organic solvents in the chemical analysis. A simple and efficient sample preparation method was developed using DLLME prior to HPLC-UV analysis for simultaneous extraction and determination of trace amounts of Non-Steroidial Anti-Inflammatory Drugs (NSAIDs) including indoprofen, ketoprofen, naproxen, diclofenac, ibuprofen, mefenamic acid, and tolfenamic acid from an aqueous sample. Optimized conditions with respect to several experimental parameters including the effects of the dispersive solvent, extraction solvent, pH and salting-out effect for the extraction of NSAIDs were established.

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발표코드: **ANAL.P-452**

발표분야: 분석화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Identification and chemical profiling of bioactive marker components from natural pigment resources using HPLC-PDA and LC-MS/MS

홍성수

경기과학기술진흥원 천연물연구팀

Pigments produce the colors that we observe at each step of our lives, because pigments are present in each one of the organisms in the world, and plants are the principal producers. Natural pigments are used in medicines, foods, clothes, furniture, cosmetics, and in other products. In this research, total 11 bioactive marker compounds such as anthraquinones (ruberythric acid and ophiohatatone B), flavonoids (butin, liquiritigenin, butein, 7,3',4'-trihydroxyflavone) and stilbene derivatives were identified in natural pigment resources (NPR), using spectroscopic analysis, high-performance liquid chromatography with photodiode array detector (HPLC-PDA) and tandem mass spectrometry (LC-MS/MS). A chemical fingerprint profiling method to display bioactive components in NPR was established and could be used for the QA/QC of the NPR and its related products.

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발표코드: **ANAL.P-453**

발표분야: 분석화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Comparison of Hydrophilic Interaction Chromatography (HILIC) and Porous Graphitized Carbon (PGC) for Efficient Glycan Separation

서나리 안현주*

충남대학교 분석과학기술대학원

Monoclonal Antibodies (mAbs) are therapeutic proteins that recognize one epitope on an antigen. Recently the importance of mAbs is growing due to their great achievement for treatment of diseases such as cancers. Especially the glycosylation of Fc fragment is essential for Fc receptor-mediated activity such as antibody-dependent cell-mediated cytotoxicity (ADCC) and complement-dependent cytotoxicity (CDC). Therefore, the characterization of glycans on antibodies is important to understand the relationship between biological activity and glycan structure. Hydrophilic interaction chromatography (HILIC) columns and porous graphitized carbon (PGC) column using liquid chromatography are widely used for glycans separation. In this study separation conditions were optimized for both columns using UHPLC / triple quadruple mass spectrometry. We have evaluated the chromatographic performance of PGC and HILIC LC using native and derivatized glycans. PGC LC can separate both neutral and acidic glycan isomers. HILIC LC, on the other hand, shows higher signal response than PGC LC (due to better MS ionization). Quantitatively, PGC LC of native glycans performs similarly with HILIC LC of derivatized glycans.

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

The Developed Technique for Efficient Identification of Glycan Isomers in NanoLC-PGC chip Q-TOF MS

서영숙 안현주*

충남대학교 분석과학기술대학원

In recent years nanoflow liquid chromatography (nano-LC)/ mass spectrometry has used to get detailed information on glycomic characterization such profiling, location, and structure of glycans. Especially, glycans with the native state are usually analyzed by PGC(porous graphitic carbon) column in LC/MS. It has competitive advantages to separate glycans owing to high resolution and sensitivity. However, it is difficult to clearly confirm glycan isomers by PGC column because the data shows both α-and β-form of glycans, resulting in observing more mass to charge peaks. In this study we find that the glycan isomers of biotherapeutic product are profiled by nanoLC-PGC chip Q-TOF MS after sample preparation combined with reduction. As the result, the efficiency of reduction is very high (98.8%) in total abundance of glycans and that of major glycans with the form of G0F1, G1F1, and G2F1 is also same. However we discovered the difference in efficiency of chemical reaction according to the types of glycans. Almost all the complex and high mannose types of glycans are reduced up to 99%. While sialylated glycans are lower than others, which is almost 91%. This developed technique can lead to efficient identification of glycan isomers in biotherapeutic product by producing reduced form of glycans.

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

Accurate applications of ESR spin trapping as a method for measuring hydroxyl radical generated by nanomaterials

정민숙 박수진 송미령 김준성*

(주)바이테리얼즈 부설연구소

In the recent decades, the use of nanomaterials has been increasing rapidly in biomedical and industrial applications. Studies on hazardous effects of nanomaterials are also increasing. Nanomaterials possess unique physicochemical properties. But many researches on hazardous effects of nanomaterials are applying conventional analytical methods without into account the physicochemical properties of nanomaterials, which can lead to misleading interpretations of data. Improving the experimental procedures needs in order to gain reliable data. In this study, we examined thoroughly the ESR spin trapping method of one of the physicochemical analysis methods. This method can provide valuable information for the prediction of ROS-mediated cytotoxicity of nanomaterials without cell-based assay at physicochemical evaluation stage. This study is expected to provide researchers to design accurate applications of ESR spin trapping method with nanomaterials and to interpret results of the toxicity studies.

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

Development of an immuno-biomaterial analyzer based on enhanced laser induced fluorescence microscopy

김영현 손경진 강다연 임흥빈*

단국대학교 화학과

In this work, an immuno-biomaterial analyzer based on enhanced compact laser induced fluorescence microscopy(LIFM) was developed to determine antibiotic, such as salinomycin. The compact LIFM has an enhanced sensitivity using the principal of the fluorescence. A mirror-coated cap in the cell holder was used for a long cell pathlength. For sample preteatment, two different kinds of nanoparticles, i.e. synthesized dye-doped core shell silica nanoparticles and magnetic nano particles (MNP) were used for fluorescent tagging and concentrating the antibiotic, salinomycin, respectively. And a synthesized dye-doped core shell silica nanoparticle included dyes of 1.68x10-22 moles.(1.68x10-22 moles/particle) We obtained the calibration curves of dye-doped silica nanoparticles we synthesized and antibiotic, salinomycin and the detection limit(LOD) of 4.2x107 particles for dye-doped silica nanoparticles we synthesized and 7pg/mL(7ppt) for salinomycin were obtained. From our experimental results, we expected to determine various antibiotics with enhanced sensitivity using our instrument we developed.

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

Profiling of lipids from lysosomal storage disease patients by nLC-ESI-MS/MS

변슬기 문명희*

연세대학교 화학과

Lysosomal storage diseases (LSD) are rarely inherited genetic disorders, developed by a deficiency of particular lysosomal proteins or enzymes. The lesions of LSD usually occur physically as the internal organs such as spleen and liver become abnormally larger by the altered metabolism of lipids and proteins. The morbidity of lyososmal storage disease is reported to be extremely low, especially in Asia, but as LSD can be fatal at extremities, studying how the profiling of lipids alter in LSD patients are important as they can served for purpose of early diagnostic test later. Among over 50 different types of LSD, Gaucher and Fabry diseases were investigated in this study. Plasma and urine from 15 healthy controls, 3 Gaucher patients, and 3 Fabry patients were drawn, and phospholipids (PL) and sphingolipids (SL) were extracted from them for further analysis. Using nanoflow liquid chromatography-electrospray ionization-tandem mass spectrometry (nLC-ESI-MS/MS), intact lipids were identified and their amounts were calculated using peak areas. A total of 125 and 106 species from plasma and urine, respectively, were identified and among these species, 18 species from plasma and 8 species from urine were increased in Gaucher patients compared to controls by greater than two-folds, while 24 and 19 species from plasma and urine, respectively, exhibited significant differences among Fabry patients.

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

Subcellular organelle fractionation of HEK293T cell by flow field-flow fractionation

양준선 문명희*

연세대학교 화학과

Organelles related with diseases have sparked great interest in biological and biomedical field. For example, when a single organelle such as mitochondria malfunctions, it can possibly lead to Alzheimer’s or Parkinson’s, Zellweger spectrum, or peroxisomal disease. As these diseases are caused by an inactivation of subcellular organelles, isolation of certain subcellular organelles from a whole cell is essential in human disease biomarker research. The separation of subcellular organelles has widely been conducted by centrifugal methods. Even though centrifugal methods are relatively simple and easy to carry out, they are time-consuming and require additional purification processes due to the low efficiency in purification. Besides centrifugal methods, fluorescence activated sorting or affinity purification methods have been developed but these methods usually require complicated pre-processing steps. Flow field-flow fractionation (FlFFF), an elution based method for size-separation of macromolecules or particles, was applied to separate the subcellular organelles within relatively short period of time, without the need of any complex preprocessing steps. The organelles from human embryonic kidney 293 T (HEK293T) cell line were separated by size in 5 minutes and during separation,and the subcellular speciesof each collected fraction was observed by Scanning Electron Microscopy (SEM). In order to analyze the organelles from each fraction, fluorescence detection along with shotgun proteomic and lipidomic analysis by nLC-ESI-MS/MS were conducted.

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

Ionic Strength Effect on Molecular Structure of Hyaluronic Acid by Flow Field-Flow Fractionation/Multiangle Light Scattering

김빛나라 문명희*

연세대학교 화학과

Sodium hyaluronate (NaHA), a sodium salt of hyaluronic acid, is a water-soluble polymer having ultrahigh molecular weight and it is widely found from nature. Due to its unusually high viscosity and elasticity at low concentration, it is widely utilized in cosmetic and pharmaceutical applications. As the properties of NaHA strongly depend on its molecular weight and their molecular structure in solution, it is important to identify the exact molecular weight distribution of sodium hyaluronate along with conformation.In this study, the effect of ionic strength on hyaluronic acid was studied by using flow field-flow fractionation (FlFFF) and multi-angle light scattering (MALS). The concentration of sodium chloride from control sample was gradually decreased by repeated procedures of ultrafiltration and solutions were collected at each ultrafiltration. In order to determine the influence of salt concentration in sample on the structure of NaHA, sodium chloride was added in one of the samples up to the final concentration of 0.3 M. The molecular weight increased as the concentration of sodium chloride in samples decreased due to aggregation. Also, the molecular weight decreased again when enough amount of salt was added. To analyze the influence of ionic strength of carrier solution in FlFFF, the experiments were carried out with different concentrations of salts in carrier solution. From the results, it was found that as the ionic strength of carrier solution decreased, NaHA became more aggregated during the separation. Experiments showed that lower ionic strength of sample induced NaHA to aggregate each other, resulting in in the increase of molecular weight and RMS radius.

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Analysis of oxidized phospholipids in Human Lipoproteins by Flow Field-Flow Fractionation and Nanoflow Liquid Chromatography-Tandem Mass Spectrometry

이주용 문명희*

연세대학교 화학과

Coronary artery diseases (CAD) refers to a disease of arteriosclerosis by accumulation of cholesterol that partially blocks the arteries, damaging heart muscles followed by other types of physical disabilities. High-density lipoprotein (HDL) and low-density lipoprotein (LDL) have been reported as the major risk factors of the CAD. Lipoproteins transport fats inside the body via bloodstream and their structures are composed of apolipoprotein and phospholipids on the outer layer and cholesterols with triglycerides in the inner layer. Oxidized lipoproteins are the uncontrolled post-modified form of lipoprotein and they have been attracting great attention since 2000 due to their characteristics of being significantbiomarkers of CAD. Various factors promote LDL to become oxidized and as lipids and proteins within LDL are altered when LDL becomes oxidized, studying the lipids from oxidized LDL is crucial.Flow field-flow fractionation (FlFFF), separation techniques for size sorting of nano to micrometer sized particles, was applied to separate the HDL and LDL from human plasma of CAD patients and healthy controls in this study. Through lipid extraction, normal and oxidized forms of phospholipids were obtained from each fractionated lipoprotein class, and they were analyzed by nanoflow liquid chromatography-tandem mass spectrometry.

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Isotope-coded carbamidomethylation for relative quantitation of liver cancer proteome using on-line mHFER-nLC-ESI-MS/MS

김진용 문명희*

연세대학교 화학과

Iodoacetamide (C_2H_4INO, IAM) is typically used for carbamidomethylation (CM) of cysteine residue of proteins prior to enzymatic digestion of proteins in which disulfide bonds are cleaved first during reduction and followed by the protection of thiol groups by alkylation. In this study, simple isotope-coded carbamidomethylation (iCCM*), a new technique for labeling cysteine residues by carbamidomethylation, was introduced using a stable isotope-coded iodoacetamide ($^{13}C_2H_2D_2INO$, IAM*) as an isotope tagging reagent for the alkylation. One of the samples was alkylated with CM method using light iodoacetamides while the other was done the same with heavy iodoacetamide. Prior to proteolysis, the samples were mixed together and using nLC-ESI-MS/MS, carbomidomethylated peptides were identified and analyzed quantitatively. Even though the developed labeling technique applies to proteins with cysteine residues only compared to other typical labeling methods, iCCM* is robust, simple, and easy to perform, resulting in higher efficiency, and the isotopde-tagged iodoacetamide is very cheap to obtain.Using iCCM* as labeling method and online-mHFER-nLC-ESI-MS/MS, lectin-bound glycoproteins from plasma samples from healthy controls and liver cancer patients were analyzed. As fucosylation to proteins is reportedly related with the development of liver cancer, fucosylated N-glycopeptides were analyzed using fucose-binding Aleuria aurantia lectin (AAL). Also, ConA was used as well as it could selectively bind to glycosylated mannose of proteins. Using two types of lectins, AAL and ConA, a total of 89 N-linked glycoproteins and 221 N-glycopeptides were identified and 73 of 221 N-glycopeptides were determined to contain the cysteine residues.

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발표분야: 분석화학
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Variations of Saponarin Content in Barley Sprouts illuminated with Four Different Light-emitting Diode (LED) Lights

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Recently, light-emitting diodes (LEDs) have been demonstrated to be efficient alternative lighting sources for plant growth and development, causing physiological and morphological variations in plants. The beneficial effects of young barley leaves are suggested to be correlated closely with the presence of potent antioxidants, especially C-glycosylflavone, saponarin, the major flavonoid of barley leaves. And it was reported that the biosynthesis of saponarin and the pathways of C-glycosylation in barley leaves could be photoregulated. In our present work, to investigate the effect of wavelength of light on the regulation of flavonoid biosynthesis in barley young leaves, the saponarin content of the young barley leaves were analyzed quantitatively with HPLC after being illuminated during sprouting period by four different LED lights, i.e. white fluorescent, blue, red, far-red light. The results show that the content of saponarin in blue light-illuminated leaves is to our surprise five times more (1152 mg/100g of dry weight of leaves) than others, while the contents of saponarin in the leaves illuminated with other wavelength of lights, i.e. white, red, far-red, and the content under even dark condition as a negative control, show no significant difference (~ 200 mg/100g of dry weight of leaves). Interestingly, the contents of saponarin are consistent with their antioxidant potentials, suggesting the fact that the light of high energy (blue, 450 nm) could cause the photoprotection mechanism resulting in the mass production of flavonoindal molecules with high antioxidant activity.

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C18 modified partially sub-1?m porous silica monolith particles as HPLCstationary phase of tremendously high separation efficiency

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Porous silica monolith particles in the partially sub-1?m range have been synthesized and modified with chlorodimethyl octadecyl silane (C18) ligand. End capping of the residual silanol groups was carried out with Hexamethyl disilazane and chlorotrimethylsilane reagent. The resultant stationary phase was packed in a 1.8mm ID X 150mm length column. Very high efficiency (N-value Ca.184000/m) along with much better resolution (6.02) were achieved when an optimized mobile phase of 70/30 acetonitrile/water, containing 0.1% TFA was used with a detection wavelength of 214nm

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Metal enhanced fluorescence on nanoporous gold leaf-based assay platform for virus detection

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In the present study, a rapid, sensitive and quantitative detection of influenza A virus targeting hemagglutinin (HA) was developed using hybrid structure of quantum dots (QDs) and nanoporous gold leaf (NPGL). NPGL film was prepared by dealloying bimetallic film where its surface morphology and roughness were fairly controlled. Anti-influenza A virus HA antibody (ab66189) was bound with NPGL and amine (?NH_2) terminated QDs. These biofunctionalized NPGL and QDs formed a complex with the influenza virus A/Beijing/262/95 (H1N1) and the photoluminescence (PL) intensities of QDs were linearly correlated with the concentrations of the virus up to 1 ng/mL while no PL was observed in the absence of the virus, or in bovine serum albumin (BSA, 1 ?g/mL) alone. In addition, it was demonstrated that this assay detected successfully influenza virus A/Yokohama/110/2009 (H3N2) that is isolated from clinical sample at a concentration of ca. 50 plaque forming units (PFU)/mL. This detection limit is 2-order more sensitive than commercially available rapid influenza diagnostic test. From these results, the proposed assay may offer a new strategy to monitor influenza virus for public health.

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Magnetophoretic immunoassay for rapid monitoring of CFP-10 in culture media of *Mycobacterium tuberculosis* by using Au nanoparticles and Magnetic microparticles

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A sandwich-type colorimetric magnetophoretic immunoassay (MPI) is introduced to monitor tuberculosis (TB) antigen, CFP-10, in cultures of Mycobacterium tuberculosis (Mtb) using nanoparticle complexes of Au nanoparticles (NPs), magnetic microparticle (MMPs), and TB immuno-moieties. The MPI can monitor the target antigen quantitatively and qualitatively within 10 min in the detection range of 101 ~ 104 pg/mL. Furthermore, the quantitative analysis of the MPI in Mtb culture showed that there was linear relationship between the concentration of the secreted CFP-10 from 106 CFU/ml of Mtb and culture time. From these data, it is suggested that the MPI analysis can carry out TB diagnosis within 3~7 days, based on antigen secretion from Mtb. These data suggest that our MPI kit is able to be applied in early TB diagnosis through detection of TB specific antigen during culture.

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O-GlcNAcylation-site Determination by CID and ETD

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O-linked N-acetylglucosamine is a reversible post-translational modification of Serine and Threonine residues on cytosolic and nuclear proteins, which regulate functions including cellular processes, gene silencing, nutrient and stress sensing, and diseases such as diabetes and Alzheimer's. However, understanding specific functions of O-GlcNAcylation in a variety of biological materials still remain challenging by the difficulty in characterization O-GlcNAc sites on proteins. Here, compositional analysis of O-GlcNAcylated peptide was carried out by identifying the peptide portion using collision-induced dissociation (CID). Further, site-determination of O-GlcNAcylation on peptide was performed by fragment the peptide backbone while intact retaining the O-GlcNAc modification from electron-transfer dissociation (ETD). We describe the unambiguous and robust strategy able to elucidate O-GlcNAcylation sites using CID and ETD combination from O-GlcNAcylated peptide standard and biological samples including O-linked N-acetylglucosamine transferase (OGT).

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All-Solid-State Phosphate(II)-Selective Electrode Using Double-layer Film of polyethylenedioxythiophene(PEDOT) Composite and Plasticized poly(vinyl chloride) Containing Tris(cyclohexyl thiourea) Amide

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경상대학교 화학과

All-solid-state phosphate(II)-selective electrodes have been constructed on a Pt disk electrode using a double-layer film of polyethylenedioxythiophene(PEDOT) composite covered with a plasticized poly(vinyl chloride) (PVC) membrane containing Tris(cyclohexyl thiourea) amide. The lower composite layer is formed by electropolymerization of EDOT in an acetonitrile containing LiClO4, and the upper PVC layer is formed by casting. The electrode shows a near-Nernstian slope, and low detection limits. The double-layer film electrode using this composite shows no overshoot and lower drift of the standard potential than both a conventional PVC electrode and a single-layer electrode using PEDOT doped with ClO4-. This is due to both the highly electrochemical activity of the lower PEDOT and the anion-exchange ability between the PEDOT and the phosphate(II)-selective membrane with active sensor elements Tris(cyclohexyl thiourea) amide.

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SERS-based immunoassay for highly sensitive bacterial toxin detection

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The time required for identification of pathogenic bacteria is a key factor in the diagnosis of infectious disease; therefore the interest in rapid bacteria detection is increasing. Conventional culture-based biochemical and serological assays are effective but suffer from disadvantages of being time consuming, costly and labor intensive proced,e. This study presents highly sensitive pathogenic bacteria detection with surface-enhanced Raman scattering (SERS) in a suspension array. Here competitive assay format has been used to detect poly-D-glutamic acid (PGA) capsule. Bacillus anthracis is surrounded by the anti-phagocytic capsule that is composed of PGA. Thus, PGA could be an effective immunoassay marker for early, specific, rapid and inexpensive diagnosis of anthracis. In this work, high affinity monoclonal antibodies (mAbs) reactive with PGA were used to construct an immunoassay platform for PGA. The assay has an extraordinarily high sensitivity, with a lower limit near sub-ng/mL. The result in this work provides a new immunoassay prototype for fast and sensitive detection of anthracis using a PGA marker.

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Synthesis and electrochemical properties of Si-CNFs composite as an anode material for Li secondary batteries

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We have performed a study on the electrochemical and structural characteristics of Si-CNFs composite which is an active anode material for lithium secondary batteries. Carbon nanofibers(CNFs) have been synthesized by Chemical Vapor Deposition (CVD) using Co and Cu catalysts. The CNFs on the surface of Si particle can provide flexible space to relieve volumetric expansion during charge. The CNFs composites on Si particles were prepared on the basis of following 2 processes; Sample 1: CNFs were grown on the simple mechanical mixture of Si particle and catalysts. Sample 2: CNFs were grown on the surface of pyrolytic carbon coated Si particles. The morphology and composition of Si-CNFs composite were analyzed by SEM and EDS measurements. Physical properties were investigated using XRD and Raman. The two different CNF-Si composite materials were evaluated as the anodic material in three electrode cells. Si-PC-CNF composite achieved the largest amount of early discharge capacity of 2118mAh/g. The suggested Si-CNFs composites can be a solution to provide higher discharge capacity and cycle-ability facilitating the 1st cycle coulombic efficiency of cheap metallic Si particles as an appropriate anodic material for Lithium batteries.AcknowledgementThis research was financially supported by the Ministry of Education (MOE) and National Research Foundation of Korea (NRF) through the Human Resource Training Project for Regional Innovation (NO. 2012026209).

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Electrochemical performance of Si-Carbon Nanofibers composite as anode material for binder-free lithium secondary battery

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The Si-Carbon nanofiber(CNF) composites were synthesized using a chemical vapor deposition(CVD) method with an iron catalyst and silicon covered Ni foam as collectors of lithium batteries. Acetylene as a carbon source was flowed into the quartz reactor of a tubular furnace heated to 700℃, and maintained for 30 min to synthesize CNFs. The morphologies, compositions and crystal quality of the prepared CNFs were characterized by scanning electron microscopy(SEM), energy dispersive spectroscopy(EDS) and X-ray diffraction(XRD). The electrochemical characteristics of Si-CNFs composites as an anode of Li secondary battery were investigated using three-electrode cell. The as-deposited Si-CNF composites on Ni foam was directly employed as an working electrode without any binder, and lithium foil was used as the counter and reference electrode. Glass fiber separator was used as the separator membrane. Two kinds of electrolytes were employed ; 1) 1M LiPF6 was dissolved in a mixture of ethylene carbonate(EC):propylene carbonate(PC):diethylcarbonate(DEC) in a 1:1:1 volume ratio, 2) 1M LiClO4 was dissolved in a mixture of propylene carbonate(PC): ethylene carbonate(EC) in a 1:1 volume ratio. The galvanostatic charge?discharge cycling and cyclic voltammetry measurements were carried out at room temperature by using a battery tester. The resulting CNF coated on Ni foam were tested as an anode for Li secondary battery and exhibited capacity near 71 mAh g^{-1} for 30cycles.Acknowledgement : This research was financially supported by the Ministry of Education (MOE) and National Research Foundation of Korea (NRF) through the Human Resource Training Project for Regional Innovation (NO. 2012026209).

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Development of versatile home-built solid-state NMR probes for special purposes

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한국외국어대학교 화학과

The solid-state NMR has been widely used for various insoluble materials like industrial polymers and biological samples, up to now. Analysis of membrane protein using solid-state NMR on lipid bilayer or bicelle for membrane-like environments, is valuable especially for a predominantly their helical secondary structure. But, most of biological lipid samples have high dielectric property due to containing large amounts of lipids, water, and salts. Since these electrical properties of lossy samples cause a loss of probe efficiency, a specific probe with high efficiency is required to study biological samples by using solid-state NMR. Development of solid-state NMR methodologies for the study of orientational information are used for the in-situ analysis of membrane protein in lipid bilayers and liquid crystalline materials in LCD panels as well as Li materials in Li ion batteries. But, these cannot be analyzed using conventional MAS equipment. Here, we present the optimized design, construction, and efficiency of a home-built 400 MHz wide-bore (WB) 1H-15N solid-state NMR probe with 5-mm solenoidal rf coil and a home-built 800 MHz narrow-bore (NB) 1H-15N solid-state NMR probe with strip-shield coil to prevent heating by high RF power for the study with lossy samples. 1H-15N 2D SAMPI4 spectra from a single crystal and membrane proteins oriented in bicelles were successfully obtained by using these solid-state NMR probe. Also, we present a home-built 500 MHz NB 19F-13C and 600 MHz NB 19F-7Li double resonance solid-state NMR probe with a flat-square coil and solenoidal coil respectively. It was the first application for the in-situ analysis of LCD panel and Li ion battery samples. These probes provide short pulses, high power capability, and good RF homogeneity.

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Optimized Expression, purification and NMR Structural Studies of syndecan-4 as a G protein-coupled receptors

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Syndecans as a G protein-coupled receptors participate in biologically important cell-to-cell and cell-matrix interactions. They have a common basic structure including modified extracellular domains, conserved transmembrane and cytoplasmic domains. One of them, syndecan-4 may affect tissue development and repair as well as the pathogenesis of numerous diseases, especially such as cancer. The transmembrane domain of syndecan-4 (Syd4-TM) consists of 25 hydrophobic amino acids and is involved in formation of dimer or oligomer of syndecan that are crucial for transduction of signals. Although the structure and function of Syd4-TM elucidated a lot of effort, Syd4-TM still have been hindered by insufficient yields and low solubility. Thus, we demonstrated optimized method for recombinant expression and purification of three kinds of Syd4-TM like wild type Syd4-TM (wt-Syd4), mutant Syd4-TM (mSyd4), and Syd4-eTC. A mutant Syd4 has a partially modified sequence of Syd4-TM and Syd4-eTC has extracellular, transmembrane and cytoplasmic domain of Syd4-TM. All peptides were released from the fusion protein, and then purified by semi-preparative reversed-phase HPLC. Enough amounts of purified Syd4-TM for the analysis was obtained from 1L of M9 minimal media under optimized conditions. Their biophysical properties of peptides were studied by circular dichroism (CD), mass spectrometry, and nuclear magnetic resonance (NMR) spectroscopy.The solution NMR studies show wt-Syd4 and Syd4-eTC form an asymmetric dimer in micelles and mSyd4 present as a monomer. Optimum structure of Syd4 was calculated by using Discovery Studio and Tilt angle was obtained by PISA Wheel based on 2D SAMPI4 solid state NMR spectra.

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Determination of polyphenolic components in *Artemisia annua L.* using high-performance liquid chromatography coupled with tandem mass spectrometry

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Artemisia annua L. is widely distributed in East Asia. The plant is used as folk medicine for the treatment of various diseases such as fever, malaria, indigestion, and has been recently disclosed its high anti-cancer effect. The principal objective of present study was to characterize pharmaceutically active component in *Artemisia annua L.* using high-performance liquid chromatography coupled with tandem mass spectrometry (HPLC-MS/MS) in negative mode.

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Growth of Carbon nanofibers on C-fiber textiles by Electrophoretic Deposition and Synthesis of SiO2-Carbon nanofiber Composites

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계명대학교 화학과

In this study, carbon nanofibers were coated with sillica layer prepared by hydrolysis of TEOS(Tetraethyl orthosilicate). The carbon nanofibers were grown by chemical vapor deposition on C-fiber textiles deposited with Ni and Cu catalyst via electrophoretic deposition. The carbon nanofibers were oxidized by nitric acid before carbon nanofiber was coated via hydrolysis of TEOS(Tetraethyl orthosilicate). Due to oxidation, hydroxyl group was created on carbon nanofiber and that was used as an activation site for SiO2. FT-IR was used to measure the effect of oxidation on functional group. The physicochemical properties of grown carbon nanofibers were investigated by SEM, EDS, BET, XRD and XPS. The structures of SiO2-coated carbon nanofibers were characterized by Raman, XPS and TEM. It is verified that catalyst particles were the most evenly deposited on C-fiber textiles by electrophoretic deposition under the condition of 8 volts for 20 minutes. Carbon nanofibers grew to an average diameter of 33nm and the SiO2 thin film is successfully coated onto the surface of grown CNFs.AcknowledgementThis research was financially supported by the Ministry of Education (MOE) and National Research Foundation of Korea (NRF) through the Human Resource Training Project for Regional Innovation (NO.2012026209).

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Detection of ochratoxin A in rice using two types nanoparticle and a lab-built LIFM based on immunoassay

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단국대학교 화학과

Ochratoxin A (OTA) is one of the mycotoxins prodeuced by Aspergillus ochraceus, Aspergillus carbonarius and Penicillium verrucosum which can be contaminated food products such as crops, coffee, wine grapes and dried grapes. OTA has shown toxicity such as carcinogenic and neurotoxic to humans. Also, OTA is immune suppressant and teratogen to animals. The European Commission has established the concentration limit of OTA in several goods (e.g., 2 ug/kg in wine, 5 ug/kg in unprocessed cereals, 10 ug/kg in dried vine fruits). we detected OTA in rice using a novel and sensitive lab-built Laser induced flourescence microscope(LIFM). We used two types nanoparticles. One is magnetic nanoparticle which is used to collect the OTA. Another is FITC dye doped nanoparticle which is used as detection probe. This approach has been widely demonstrated to provide superior analytical performance and short assay times.

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NORMAL-PHASE 2 COLUMN MODE HIGH PERFORMANCE LIQUID CHROMATOGRAPHY SEPARATION FOR CRUDE OIL ANALYSIS

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경북대학교 화학과

The petroleum industry takes a number of chromatographic techniques for the evaluation of the crude oils for hydrocarbon group type composition. Among these techniques, high performance liquid chromatography (HPLC) is the widely used method for determining hydrocarbon group types and further differentiation of aromatic types. The purpose of this study is separate oil by the number of aromatic ring types. Separation is carried out by using 6-port valve and normal phase mode column. 2 columns, a propylaminocyano (PAC) and a dinitroaminopropyl column (DNAP), are separate the oil sample into 6 groups : Saturates, 1-4 aromatic rings, Polars. Five main chromatographic peaks were observed as the separation method. After this step, each fractions are analyzed by APPI(+) Quadrupole orbitrap MS. This report represents the utilize of 2 columns and developing optimized method for oil analysis.

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MEASUREMENT OF SESAMIN IN VEGETABLE OIL USING 1H NUCLEAR MAGNETIC RESONANCE SPECTROSCOPY

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고려대학교 화학과 [1]한국과학기술연구원(KIST) 특성분석센터

An NMR method is reported for the determination of sesamin in vegetable oil. The intensity of the well-resolved H2′ sesamin signal resonating at approximately 5.95 ppm is strongly correlated with the amounts of other types of vegetable oils present in the adulterated sesame oil using the relationship, $y = 4.020x + 1.516$ ($r2=0.9967$). The H2′ peak intensity of sesamin was measured for sesame oil extracted directly from the millsourced sesame seeds because the sesame oils purchased from local markets could be adulterated. Additionally, the oils used were obtained from the seeds native to China and the Republic of Korea, because the sesamin concentrations may vary from region to region. The proposed 1H NMR method allows for the simple identification and determination of cheaper vegetable oils used as adulterants in sesame oil. High-performance liquid chromatography was used to confirm the validity of the results obtained by NMR.

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Application of ^{13}C CP-MAS NMR to study chemical transformations in downed logs and snags of mixed boreal species during decomposition

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Snags and downed logs are substantial components of the detrital carbon pool in boreal forests. Effects of their decomposition on chemical and physical characteristics of the forest floor remain relatively unknown. The main objective of this study was to characterize chemical transformations of decaying logs and snags of common tree species in the boreal mixed wood forest. Logs and snags from a wide range of decay classes were sampled and analyzed by solid-state ^{13}C nuclear magnetic resonance spectroscopy. Little or moderate chemical changes appeared in fresh and moderately decayed snags and logs, but in well-decayed logs, substantial degradation of carbohydrates and increases in lignin concentrations occurred. Deciduous species had initially more carbohydrates than coniferous species, but decomposition narrowed their differences, and in well-decayed logs, species differed mainly in terms of their lignin concentrations. Well-decayed deciduous logs reached very low wood densities, and their integration into the forest floor and long-term preservation remains questionable. In contrast, chemical composition of well-decayed coniferous logs resembles that of lignic forest floor (i.e., forest floor originating from deadwood decomposition), with preserved lignins, carbohydrates, and alkyl carbon compounds. Decomposed coniferous wood thus contributes to chemical heterogeneity of the forest floor, possibly promoting diversity of decomposers as well as carbon retention in soils.

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Large scale splitter-less FFD-SPLITT fractionation: Effect of flow rate and channel thickness on fractionation efficiency and sample recovery

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SPLITT fractionation (SF) allows continuous (and thus a preparative scale) separation of micro-sized particles into two size fractions. SF is usually carried out in a thin rectangular channel with two inlets and two outlets, which is equipped with flow stream splitters at the inlet and the outlet of the channel, respectively.A large scale splitter-less gravitational SF (GSF) system had been designed and assembled, which was designed to avoid the flow stream splitters and to increase throughput (*TP*), thus is operated by the full feed depletion mode (FFD-GSF). There is only one inlet through which the sample is fed, and no carrier liquid fed into the channel, preventing dilution of the sample suspension. The effects of *TP* and the channel thickness on the fractionation efficiency (*FE*, number % of particles that have the size predicted by SPLITT theory) and the sample recovery of FFD-GSF was investigated using industrial polyurethane (PU) latex beads. Water containing 0.1% FL-70 (dispersing agent) and 0.02% sodium azide (bactericide) was chosen as the carrier liquid. The sample loading was varied from 4.2 to 7.2 L/hr with the sample concentration fixed at 0.02%, and the GSF channel thickness was varied from 900 to 1300 μm. Particles fractionated by GSF were collected and monitored by optical microscopy (OM). Sample recovery was determined by collecting the fractionated particles on a 0.45 μm membrane filter. The new splitter-less FFD GSF system seems to have a potential to become useful for large scale-separation of micron-sized industrial particulates.

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Synthesis and Characterization of Highly Stable Quantum Sized Silver Nanoclusters Protected with 3-Mercapto-1-propylsulfonate

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연세대학교 화학과

In recent years, owing to the abundance of the materials, low cost and interesting optical properties, compared to gold nanoclusters, silver nanoclusters (AgNCs) became one of the most extensively studied fields. However, the low stability of the AgNCs has always been a big challenge until now. In this presentation, we present the synthesis and characterization of a highly pure and very stable, water soluble AgNCs protected by 3-mercapto-1-propylsulfonate ligands (MPS). The synthesis was carried out at 0 °C by reducing AgNO3 with sodium borohydride in the presence of MPS ligands. Thus prepared cluster mixture was further purified by poly-acrylamide gel electrophoresis (PAGE), which isolated two major clusters. These two AgNCs were found to be $Ag_{44}(MPS)_{30}$ and $Ag_{32}(MPS)_{19}$, identified by electrospray ionization mass spectrometry (ESI-MS) and matrix-assisted laser desorption/ionization time of flight (MALDI-TOF). These clusters were water soluble and found to be stable at room temperature for more than a month. The presence of sulfonate terminal groups at the end of the ligands enabled facile modification of the anionic clusters by ion-pairing with functional cations. Consequently, it was possible for water soluble AgNCs to phase-transfer to organic phase for further electrochemistry studies.

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Ionic Liquid of a Au_{25} Nanocluster Modified with Glucose Dehydrogenase for Glucose Sensing Application

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Recently, thiolate-protected gold nanoclusters containing less than a few hundred of core atoms have attracted much research interest due to their unusual physical and chemical properties. In particular, Au_{25} nanoparticles (~1.1 nm) are very stable nanoclusters that exhibit unique electrochemical and optical properties. The redox-active behavior and excellent catalytic activity of Au_{25} make it an ideal candidate for electrochemical sensing applications. In this poster, we demonstrate the electron transfer between the glucose dehydrogenase (GDH) enzyme with redox-active Au_{25}nanoclusters ionic liquid film for an oxygen-free biosensing of glucose. Highly viscous room temperature ionic liquid, i.e., 1-decyl-3-methylimidazolium (DMIm) was utilized to entrap both the negatively charged (3-mercaptopropyl) sulfonate stabilized Au_{25}nanocluster (MPS-Au_{25}) and GDH to develop a stable film through electrostatic interactions. The cyclic voltammogram of the GDH-DMIm-Au25 electrode exhibited well-defined and reversible redox peaks corresponding to first ($Au_{25}^{0/1-}$)and second ($Au_{25}^{+1/0}$) oxidation states of Au_{25} nanoclusters. For the successive additions of glucose, the proposed sensor showed enhanced oxidation peak currents, suggesting the Au_{25} mediated catalysis for glucose oxidation. In addition, the electron transfer dynamics in modified electrode was investigated as a function of Au_{25} to manifests the dual role of Au_{25}both as an electronic conductor and a redox mediator.

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Size-Dependent Photocatalytic and Electrocatalytic Activities of ZnO-Au Composites

김현지 이용진 이동일*

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Semiconductors have been one of the most used materials as photocatalysts, due to their outstanding ability to absorb solar energy and to convert it to chemical energy. Additionally, through these past few years, semiconductors modified with nanoparticles have been vastly used for photocatalyst studies because of their high charge separation properties and increased catalytic activities. This poster describes size effects on photocatalytic activities of ZnO nanoparticles coated with gold nanoparticles with diameters of 1.1, 1.6, and 2.8 nm for degradation of organic dyes, thionine and azobenzene. Whereas the photocatalytic activity of ZnO-Au composites for the reduction of thionine increases with the size of gold nanoparticles, the reduction of azobenzene was only observed with composites modified with 2.8 nm gold nanoparticles. To understand the origin of this difference, electrocatalytic activities of these composites were compared, which showed the same size effect. The electron transfer dynamics in the composites and the reduction dynamics of azobenzene were investigated using time-resolved fluorescence studies.

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Restriction Fragment Mass Polymorphism Assay for Human Papillomavirus by Desorption Electrospray Ionization (DESI) Mass Spectrometry

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Persistent human papillomavirus (HPV) infection is the primary cause of cervical cancer, and there is an increasing need for more accurate, broad-spectrum and high-throughput methods for HPV genotyping to use as a screening tool for early detection.[1,2] The restriction fragment mass polymorphism (RFMP) assay based on nucleic acid target amplification and mass detection using matrix-assisted laser desorption ionization time-of-flight (MALDI-TOF) mass spectrometry was developed and adapted to HPV genotyping for evaluating the clinical utility.[3] Unlikely MALDI, desorption electrospray ionization (DESI) is an ionization method in ambient condition and there is no approach to analyze HPV genotyping by DESI mass spectrometer. We designed for HPVs assay by DESI mass spectrometry and tested its feasibility to diagnose cervical cancer. [1] Lanoni et al., Diagn. Mol. Phthol. 10: 200-206 (2001)[2] Munoz et al., N. Engl. J. Med. 357:1579-1588 (2003)[3] Lee et al., J. Med. Virol. 83: 471-482 (2011)

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Synthesis and Characterization of Atomically Precise Silver Nanoclusters Protected with Thiolate Ligands

서은영 표경림 이동일*

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In recent years, quantum-sized noble metal nanoclusters have made a significant impact in wide range of applications such as electrochemical sensing, photocatalysis, optoelectronics, energy conversion and biomedical applications. However, synthesis and isolation of ultra-small silver nanoclusters (AgNCs) have proven to be a challenging task due to the complexity of their preparation and insufficient stability. This poster focuses on synthesis, isolation and characterization of AgNCs protected with L-glutathione (SG) i.e., $Ag_{32}(SG)_{19}$ and with p-mercaptobenzoic acid (p-MBA) i.e., $Ag_{44}(p\text{-}MBA)_{30}$ as verified by mass spectrometry. The cluster synthesis was carried out by reducing silver nitrate ($AgNO_3$) using sodium borohydride ($NaBH_4$) in the presence of stabilizing ligands either with SG or p-MBA. Further, the separation of AgNCs was performed using polyacrylamide gel electrophoresis (PAGE) based on charge to mass ratio of individual AgNCs. The successful preparation of $Ag_{32}(SG)_{19}$ and $Ag_{44}(p\text{-}MBA)_{30}$ nanoclusters was confirmed by UV-Vis spectroscopy, electrospray ionization mass spectrometry (ESI-MS) and matrix assisted laser desorption/ionization time-of-flight mass spectrometry (MALDI-TOF MS) studies. Moreover, our photoluminescence studies revealed $Ag_{32}(SG)_{19}$ exhibits much higher quantum yield as compared to $Au_{25}(SG)_{18}$.

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Functional group position effect on the resolution of fendiline analogues on a crown ether-based chiral stationary phase

이가람 성지영 안성애 현명호*

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Fendiline is medical supply used in the treat of coronary heart disease. It is also sub-sorted lipophilic calcium antagonist group. It binds to the calcium channel and to calmodulin with rather similar affinities like smooth muscle relaxation, inhibition of the trance membrane calcium current. Some of fendiline analogues were found to increase the concentration of cytoplasimc Ca2+ in borine parathyroid cells and inhibited parathyroid hormone(PTH) secreation. Fendiline is a chiral medication. So it occurs different biological efficacy in chiral condition like human body. All of these effect were found to the stereoselective, the (R)-enantiomer being 10-to 100-fold more potent them the (S)-enantiomer. Thus, resolution of fendiline and its analogues is really significant.In this study, we synthesized fendiline and its analogues and resolved them on chiral stationary phases(CSP) based on (+)-(18-crown-6)-2,3,11,12-tetracarboxylic acid. The chiral resolution was found to the affected significantly by the position of the functional group on the phenyl ring at the chiral center of fendiline analogues.

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Liquid chromatographic resolution of N-(3,5-dinitrobenzoyl)-α-amino acid derivates on a new chiral stationary phase

조은솔 김희은 **RajalingamAgneeswari** 현명호*

부산대학교 화학과

Chromatographic resolution of the two enantiomers has been known as one of the most accurate, convenient and economic means for the separation of the two enantiomers.In this study, we prepared a new chiral stationary phase (CSP) based on (+)-(18-crown-6)-2,3,11,12-tetra-carboxylic acid and (R)-1-(α-naphthyl)ethylamine. The new CSP was applied to the resolution of various N-(3,5-dinitrobenzoyl)- α-amino amides and esters. The chromatographic resolution results were found to be dependent on the stereochemistry of the two chiral units used for the preparation of the CSP.

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Separation of the two enantiomers of N-(3,5-dinitrobenzoyl)-α-amino amides and esters on a new chiral stationary phase

전희영 이가람 **RajalingamAgneeswari** 현명호*

부산대학교 화학과

A new liquid chromatographic chiral stationary phase (CSP) containing two chiral units such as (+)-(18-crown-6)-2,3,11,12-tetracarboxylic acid and (S)-1-(α-naphthyl)ethylamine was prepared. The new CSP was applied to the resolution of N-(3,5-dinitrobenzoyl)-α-amino amides of esters. From the chromatographic resolution results we concluded that the chiral recognition is dependent on the chirality of the two chiral units utilized for the preparation of the CSP.

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Exploration of Resazurin-like reduction mechanisms caused by glucose oxidase based enzymatic reaction

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Resazurin (Rz) is a common anaerobic indicator and it has also been used for pointing the change of pH value and redox. We build an enzymatic system consist with glucose oxidase and glucose to exploring the reaction mechanism of Rz. As we all known, the glucose oxidase can catalyze glucose with the generation of electron. The reaction is as follows:Glucose+GOD/FAD→Gluconic acid+GOD/$FADH_2$
GOD/$FADH_2$→GOD/FAD+$2H^+$+$2e^-$
After adding Rz to our enzymatic system, the color of the solution changes from blue to pink with the reaction carried out and the maximum absorbance of the solution changes from 600 nm to 572 nm [1]. However, more interesting is that after several hours, the color of the solution star to fad and finally changes to light yellow, which was named as dihydroresorufin (HRf) and it exhibits two new absorbance bands at 480 and 402 nm [2]. The entire phenomenon is caused by the electron produced by the enzymatic reaction and the electron will lead to the two steps reduction of Rz. Based on this reaction, to exploring the mechanism of the reaction and realize the detection of glucose, UV-vis is not enough to complete the research to this reaction. So surface enhancement raman spectroscopy (SERS) was utilized for further studying the whole procedure and explore a new simple method for the detection of glucose.

[1] A. Balcerzyk, G. Baldacchinoa, Analyst, 2013, 00, 1-3.
[2] A. Mills, J. Wang and M. McGrady, J. Phys. Chem. B, 2006, 110, 18324-18331.

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Untargeted metabolite profiling study in a rat model induced myocardial infarction

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Myocardial infarction (MI) is a fatal heart failure, which associated with ischemic necrosis of cardiac muscles. Currently, many researches are in progress to investigate the biological pathways and identify biomarkers for disease, but there still little known about temporal changes including metabolite levels after MI. In this study, we applied 1H nuclear magnetic resonance (NMR) spectroscopy coupled with multivariate statistical analysis to perform metabolic profiling of sera in a rat model of myocardial infarction produced by ligation of the left coronary artery. The acquired data was analyzed by principal component analysis (PCA) and partial least squares discriminant analysis (PLS-DA). The obvious differences in the initial stages 1hr and 1day groups compared with control group were observed. Particularly, metabolites involved in energy metabolism such as glucose, lactate, pyruvate, valine, leucine and isoleucine were distinct differences among the groups. These results suggest that 1H NMR based metabolic profiling of serum in rat model of MI may be useful for the effective diagnosis of MI and a further understanding of its pathogenesis.

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In situ and sequential monitoring of thermoreversible behavior of multilayer films with different sizes of Au nanoparticles by surface plasmon resonance spectroscopy

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Thermoreversible behavior of surface plasmon resonance (SPR) is reported for various sizes of Au nanoparticles (NPs; 4, 18, and 57 nm) dangled from poly(N-isopropylacrylamide) (PNIPAm) in the solid film regime. The formation and thermal behavior of the polymer layers and NP layers were characterized by SPR spectroscopy. Changes in the thickness of the polymer film depending on temperature are expressed as shifts in the surface plasmon angle. Adsorption of Au NPs with different sizes to form the top layer results in significant amplification of the SPR signal because of the interaction of the propagating and localized SPR. SPR measurements were performed over a complete temperature cycle from 28°C to 40°C and back in order to obtain a thermal hysteresis curve. Molecular dynamics (MD) simulations were carried out in order to reveal the mechanisms involved in the formation of the Au NP layer on the temperature-sensitive polymer. This research will potentially provide basic fundamental resources for the study of the thermally dependent behavior of optoelectronics and electronics, as well as for further development of platforms for biomedical sensing and actuators.

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Development of novel multi (pH-electro) responsive chitosan based nanocomposites

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Stimuli responsive polymeric nanocomposites that respond to external stimuli such as exposure to light, heat, chemicals, etc with a change of at least one of their properties have gained significant importance from researchers both in academia and industry. Motivated by the objective to create, pH and electroresponsive materials, we developed a new approach to prepare chitosan (CS) based polymer nanocomposite (PNC). We prepared the new PNCs from CS, carbon nanostructure (CNS), polyaniline (PANI) and poly (acrylic acid) (designated as CNS-CS-PAA-PNC). In the first step, CNS-CS-PAA-PNC was prepared by the free radical grafting and cross-linking reactions among CNS, CS and PAA. In the second step, PANI was distributed into the IPN gel via impregnation of aniline monomer and oxidative polymerization. For comparison, the CS-PAA-PNC and CS-PANI-PNCs were prepared. FTIR spectroscopy and scanning electron microscopy were used to investigate structure and morphology of PNCs. This work is a part of efforts to develop new and efficient carbon nanomaterials included functional gel adsorbent for the efficient removal of environmental pollutant ions.

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Preparation of new magnetic nanocomposites incorporated with iron oxide and gold nanoparticles

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Looking for new strategies with improved efficiency and to use magnetically responsive structures has attracted attention of many researchers. In this work, we describe the design and preparation of new functional material consisting of magnetic particles embedded within polymer microparticles. A facile approach has been established for the synthesis of a new functional magnetic composite (MNC). In the MNC, iron oxide (IO) nanoparticles and gold nanostructures (AuNS) are distributed in a polymer gel matrix. The MNC is designated as IO-AuNS. The structure and morphologies of the as prepared materials (MNCs) were characterized.

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Preparation of new nanocomposites based on Sulfonated poly(ether ether ketone) and incorporated with inorganic filler oxide

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Sulfonated polyether ether ketone (SPEEK) is an inexpensive polymer electrolyte and it possesses satisfactory mechanical properties, thermal properties and good chemical stability. However, the proton conductivity of SPEEK membranes mainly depends on water content, and limits high temperature fuel cell operation. Incorporation of nanosized inorganic filler materials into the polymer matrix can influence the properties of the parent polymer, such as proton conductivity, mechanical and thermal stability. In the present study, the influence of graphene (GF) and metal ioxide (MO) fillers on a SPEEK polymer composite has been investigated. The new materials were designated as SPEEK/GF/MO nanocomposites (NCs). SPEEK-NCs, fabricated by a solution casting method, were characterized by examining their surface morphology, and their ion exchange capacity, water uptake and proton conductivity have been investigated. Degree of functional particles (GF and MO) inclusions in SPEEK was ascertained by Fourier transform infrared spectroscopy and X-ray diffraction analysis. The SPEEK/GF/MO-NCs were characterized for morphology, thermal and proton-exchange properties. The membrane stability, i.e. liquid uptake in water and in aqueous methanol solution, oxidative stability as well as mechanical and thermal stability was tested.

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Synthesis and characterization of new poly(aminophenyl boronic acid) nanocomposites

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In this investigation, a new strategy was proposed based on the specific binding of carboxylic acid functionalized carbon nanostructures with 3-aminophenylboronic acid to generate CNS grafted poly(aminophenyl boronic acid) (CNS-g-PAPBA) nanocomposites. CNS was linked to PAPBA due to their high specific surface area, excellent electronic conductivity, outstanding chemical and electrochemical stability. The CNS-g-PAPBA nanocomposite was found to show different morphology, electrical properties, thermal behavior and structural characterization in comparison to the nanocomposites prepared without incorporation of CNS. The morphology of CNS-g-PAPBA was investigated by using field emission electron microscopy. UV-visible spectroscopy, thermogravimetric analysis, Fourier transform infrared spectroscopy, and X-ray diffraction analysis were used for characterization. The CNS-g-PAPBA nanocompsite is a promising material for glucose sensor.

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QSPR models for the melting point of diverse organic compounds with applicability domain definition

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Melting point (MP) is one of the most important physicochemical properties of organic compounds, which has numerous applications in biochemical and environmental sciences. It also affects the toxicity of a compound due to its relationship with other physicochemical properties such as vapor pressure and aqueous solubility. Therefore, MP can be directly related to the chemical structure of diverse organic compounds. The MP of many organic compounds can be predicted by previously developed QSPR tools, as well as experimental results. For the specific compounds, however, like high energy molecules, there are still some limitations, the lack of experimental data. The use of in silico methods, such a QSPR model with well-defined larger coverage of applicability domain, is a good alternative to reduce the time and costs of experiments for measuring MP of diverse organic compounds.In this study, a dataset of 10,658 solid compounds was collected from different MP data sources, mostly consisting of compounds not only from common organic molecules but also from some high energy molecules. The multiple linear regression (MLR), k-nearest neighbors (k-NN) and support vector machine (SVM) models for MP dataset were developed based on meaningful 2D descriptor set. All the models from combined set of descriptors based on forward selection and bootstrapping validation methods were shown to have acceptable predictabilities. Y-scrambling and internal validations were applied to check the chance of correlation and verify the validity of models. To improve the performance of each model, the parameter conditions of k-NN and SVM models were varied in a systematic grid search and the consensus models of its model were performed. Finally, applicability domain of MP prediction model was defined based on descriptor of training set. This research is supported by Civil Military Technology Cooperation Center as "Dual Use Technology Program".

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QSPR models for the boiling point of diverse organic compounds with applicability domain definition

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Boiling point (BP) is one of the most important physicochemical properties of organic compounds, which is usually used to estimate many other properties such as critical temperatures, flash points and enthalpies of vaporization. Accordingly, BP is one of the most important thermal properties to characterize and identify the target compounds, and it can be directly related to the chemical structure of diverse organic compounds. The BP of many organic compounds can be predicted by previously developed QSPR tools, as well as experimental results. For the specific compounds, however, like high energy molecules, there are still some limitations, the lack of experimental data. The use of in silico methods, such a QSPR model with well-defined larger coverage of applicability domain, is a good alternative to reduce the time, costs, and risk of experiments for measuring BP of diverse organic compounds.In this study, a dataset of 6,253 liquid compounds was collected from different BP data sources, mostly consisting of compounds not only from common organic molecules but also from some high energy molecules. The multiple linear regression (MLR), k-nearest neighbors (k-NN), artificial neural networks (ANN) and support vector machine (SVM) models for BP dataset were developed based on meaningful 2D descriptor set. All the models from combined set of descriptors based on forward selection and bootstrapping validation methods were shown to have acceptable predictabilities. Y-scrambling and internal validations were applied to check the chance of correlation and verify the validity of models. To improve the performance of each model, the parameter conditions of k-NN and SVM models were varied in a systematic grid search and the consensus models of its model were performed. Finally, applicability domain of BP prediction model was defined based on descriptor of training set. This research is supported by Civil Military Technology Cooperation Center as "Dual Use Technology Program".

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Electrochemical and structural study of LiFeBO$_3$: a cathode material for Li secondary battery

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울산대학교 화학과

LiMBO$_3$ (M = Fe, Co, Mn) has been identi?ed as an promising new cathode material for Li-ion batteries. Especially, Lithium iron borate (LiFeBO$_3$) is a desirable cathode material for lithium-ion batteries due to its high theoretical capacity (220 mAh g^{-1}) and its favorable chemical component, which are abundant, inexpensive and non-toxic. The crystal structure of synthesized samples was characterized by X-ray diffraction, scanning electron microscopy, and transmission electron microscopy. The electrochemical measurement of the synthesized sample was performed with half cell and structural investigations of cathode material have been performed by ^{11}B MAS NMR.

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Citric acid-assisted combustion synthesis and characterization of nano-sized $LiFePO_4$ cathode materials by using different iron source as cathode material for Li-ion batteries

안지은 박지현 이영일*

울산대학교 화학과

Novel powder synthesis technologies provide opportunities to develop high performance, low-cost cathode material. In this report the nano-sized $LiFePO_4$(LFP) cathode materials have been synthesized by solution-wet route (SR) by using four different iron source as cathode material.. Depending on which iron source of preparation is used, the material is obtained either free of any detetable impurity or include impurity phases. They were characterized by TGA/DTA, XRD, TEM, SEM and EDX techniques. The electro-chemical properties of as prepared LFP were systematically measured by cyclic voltammetry and constant current charge and discharge cycling test.

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Application of Atmospheric Pressure chemical Ionization Hydrogen/Deuterium Exchange Mass Spectrometry for the Speciation of functional groups of Nitrogen Compounds

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경북대학교 화학과

Speciation of functional groups of nitrogen compounds using atmospheric pressure photo ionization hydrogen/deuterium exchange mass spectrometry has reperted earlier. It demonstrated that the functional groups of nitrogen compounds containing primary, secondary and tertiary amines, as well as pyridine and pyrrole groups were distinguishable through this method. In this study, we have applied atmospheric pressure chemical ionization hydrogen/deuterium excahnge mass spectrometry to speciation of nitrogen isomers. It was observed that nitrogen containing compounds mainly produced an D+ attached ion of which hydrogens in the functional groups were exchanged by deuterium. This result suggests that atmospheric pressure chemical ionization hydrogen/deuterium excahnge mass spectrometry can be a useful method for the speciation of nitrogen functional groups. Further, it could be used to study complex compounds containing nitrogen compounds such as crude oil.

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Development of Electrospun new chitosan blend nanofibers

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Nanoscale films and polymer membranes (mats) often exhibit enhanced efficiency because of their large specific area and superior mechanical properties. Such polymer mats can not only present the specific physicochemical properties of the polymer but can also benefit from the physical characteristics of nanoporous membranes. The fabrication of chitosan (Ch) polymer nanofibers has gained much attention in recent years because of chitosan's unique properties that lead to potential applications in many areasIn order to provide spinability, a number of researchers have combined Ch with synthetic, water-soluble, biocompatible support polymers such as PVA poly(vinyl alcohol). Our approach employs PVA as a support polymer in order to facilitate electrospinnability. Ch and graphene(GF) were blended to obtain nanofiberswith PVA as a supporting polymer at various volumetric ratios by electrospinning method.The two types of blends, Ch/PVA/ GF and Ch/PVA, were prepared in various concentration ratios and their nanofibers were obtained with a fixed distance from the needle/syringe set-up. Chemical compositions and molecular interactions among nanofiber blend components were determined using Fourier transform infrared spectroscopy (FTIR). The properties of the PMCh/PVA/PEDOT blend electrospun nanofibers at various volume ratios were examined using SEM and FTIR. In each step of studies the properties of Ch/PVA/GF were compared with Ch/PVA nanofibers.

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Synthesis and structural features of new spinel based nanomaterials

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The synthesis of ion exchange materials was attempted to find new nanomaterials with structure suitable for many purposes such as water purification and metal extraction from water resources. Li ion migration dynamics in the bulk and at the surface of alloys are important aspects to be considered in these respects. Vacancy mediated Li migration and interstitial Li migration can be considerd. In the present work, new spinel based nanomaterials were prepared by a combination of chemical synthesis and electrospinning. The prepared materials has been characterized by Field emission electron microscopy, X-ray diffraction, X-ray fluorescence, Fourier transform Infrared Spectroscopy, X- ray photoelectron spectroscopy and thermogravemetric analyses. Finally, the application of the prepared materials for the removal of lithium ions in terms of capacity measurements was performed

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Laser-Induced Breakdown Spectroscopy Analysis of Sulfur in Edible Salts

이용훈* 남상호 공용득 배동선

목포대학교 화학과

Sulfur is contained in edible sea salts in form of sulfate ions. Typically, the concentraion of sulfur in the sea salts is in the range between 0.1 and 1 wt.%. The sulfate ions in the feedstock sea salts is transformed to sulfides during the roasting process. The sulfides in the roasted salts have been found to be highly beneficial to human health. Therefore, the analysis of sulfur in edible salts, such as sea salts and bamboo salts, is very important to choose better feedstock salts for producing high-quality bamboo salts and also to analyze the quality of produced bamboo salts. Laser-induced breakdown spectroscopy (LIBS) can perform elemental analysis with little to no sample preparaion. This makes LIBS strong as a rapid quality monitoring tool in many industrial applications. We applied LIBS for quantitative analysis of sulfur in edible salts. A Nd:YAG laser beam was focused on the surface of salt pellets. The S II lines around 540 nm were observed with increased signal-to-noise ratio by flowing He gas. Univariate and multivariate data analyses were performed to obtained reliable calibration results.

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Analysis of derivatized an organic compound on silica surface by using TOF-SIMS

진종성* 김도연 김종욱

한국기초과학지원연구원 부산센터

We have been studied the synthesizing of helical silica nanotubes via polycondensation of tetraethoxysilane on self-assembled structures that were composed 1,2-diphenylethylenediamine based neutral and cationic gelators. On the other hand, a chiral stationary phase prepared by bonding (+)-(18-crown-6)-2,3,11,12-tetracarboxylic acid to silica gel was successfully employed in resolving various chiral compounds.In this study, we analyzed the helical silica nanotubes and derivatized chiral stationary phases by using TOF-SIMS. We discussed products of each steps for the derivatized organic compound on the silica surface in order to confirm the reactions.This work was supported by the grant No. R0001026 from the Ministry of Trade, Industry and Energy and Busan Metropolitan City, Korea.

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[발표취소] Monitoring of Atmospheric HX/X_2 Gases by Diffusion Scrubber Coupled Ion Chromatography

유승민 이동수*

연세대학교 화학과

발 표 취 소
본 논문은 발표취소된 논문입니다.

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Chiral separation by new phenylalaninol and tryptophanol derived chiral stationary phases

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경북대학교 화학과 [1]경북대학교 화학교육과

본 연구실에서는 phenylglycinol, leucinol, alaninol 등 다양한 키랄 정지상을 개발하였으며, 다양한키랄 물질에 대해서 성공적인 분리효능을 보였다 1,2. 본 연구에서는 amino alcohol 중 phenylglycionol 과 유사한 phenylalaninol 과 indole 기를 가지는 tryptophanol 을 출발 물질로 하여 π-산성작용기를 가지는 3,5-dinitrobenzoyl 유도체 정지상을 합성하였다. Phenylalaninol 은 phenylglycinol 과 비교하여 phenyl 기의 위치가 다르며, tryptophanol 은 phenylalaninol 과 비교하여 indole 기를 지닌다. 이 차이를 통하여 어떠한 작용기가 키랄 분리에 효과적으로 이용되었는지 비교하기 위하여 의약품을 포함한 다양한 키랄 시료를 분리 분석하여 앞서 제조된 키랄 정지상에서 각 시료들의 분리 패턴(분리 순서, 분리 인자 및 용량인자 등)을 비교하였다.1 J.J.Ryoo et.al. chirality 14, 329, 20022 J.J.Ryoo et.al. Microchemical J. 63, 128, 1999

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Phase Separation in Diblock Copolymer and Blend Homopolymer films Measured by Nanoscale Analytical Techniques

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한국과학기술연구원(KIST) 특성분석센터

As the annealing temperature is changed, the morphology of block copolymer film is changed. The annealed copolymers form the ordered arrangement, which called microphase separation normally observed in block copolymers. In this study, symmetric diblock poly(deuterated styrene-*b*-methyl methacrylate) (dPS-*b*-PMMA) and symmetric diblock poly(deuterated styrene-*b*-ethyl hexylacrylate) (dPS-*b*-PEHA) were used to investigate microphase separation in copolymer films. Blend homopolymers were also used to compare their nanostructures on the surface with those of diblock copolymers. Block copolymer and blend homopolymer films were annealed in the vacuum oven to observe microphase separation. Atomic Force Microscopy (AFM) and Time-Of-Flight Secondary Ion Mass Spectrometry (TOF-SIMS) were used to obtain the nanostructural information of the diblock copolymers and the blend polymers. The tapping mode AFM results provided information about the surface morphology, microphase-separated structure, and thickness of the films according to the annealing condition and copolymer concentration. The TOF-SIMS results provided the composition information for lamellar structure of the diblock copolymer films. Accurate surface structure information on the diblock copolymers and blend homopolymers was obtained by the combined images of TOF-SIMS and AFM.

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Identification of Dyes in Archaeological Textiles by TOF-SIMS and Raman Spectroscopy

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Analytical identification of dyes in archaeological textiles is an indispensable task for conservation research and restoration of ancient remains. However, excavated textiles were changed in the color because of burial environment through centuries and gradually fade after excavation. Furthermore, the identification of dyes in cultural heritage objects is very difficult. Several studies have been dedicated to the identification of dyes in various types of textiles by using various analytical techniques such as LC-MS, GC-MS, and HPLC. In most of these techniques, the dyes should be extracted from the textile fibers before the analysis of the colorant. In addition, a large amount of textile material is required in order to obtain a sufficient amount of dye. Therefore, non-destructive and high sensitivity techniques are needed to solve these problems. In this study, Surface analytical instruments such as TOF-SIMS, XRF, and Raman spectroscopy were used for dye detection and their results were compared. Prior to analysis of excavated textiles, we identified characteristic peaks of dyes such as indigo, alizarin, purpurin, curcumin and quercetin using TOF-SIMS and Raman spectroscopy. After the methodology to determine the dyes in the textiles was established, surface analytical techniques were also carried out on ancient textiles from Korean tombs and Mongolian area.

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Bacteria Swimming Force Detection by Atomic Force Microscope

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Numerous bacteria have flagella that make them capable of swimming through water-based environments. The bacterial flagella are driven by a reversible rotary nano-machine made up of protein. The engine is powered by proton- or the sodium-motive force. A method to measure bacteria motion should be a useful tool for various questions of bacterial movement. However, the detection of bacterial motion is difficult because bacteria are too small that they are bounced around randomly by water molecules. Here in, we showed a new technique for measuring the motion of single bacterial flagellum by AFM with a modified cantilever. The reconstruction of AFM probe was carried out by FIB(Focused Ion Beam) procedure and hydrogel coating of the cantilever. Bacterial motions were characterised by atomic force microscope, nanoindentation mode, confocal microscope and scanning electron microscope.

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Trace Level Anion Analysis Using Carbonate Eluent by Suppressed Ion Chromatography

최혜미 이동수*

연세대학교 화학과

Carbonate/bicarbonate aqueous solution being the first and still most widely used eluent for suppressed anion chromatography, it is not particularly useful for trace level analysis because it has poor detection limits compared to hydroxide eluent. Poor detection limits is stemmed from high background conductivity of suppressed eluent of carbonic acid. Background conductivity of carbonate eluent runs 15 ~ 20 uS/cm while that of hydroxide eluent does less than 0.5 uS/cm. In this presentation, we will show a promising method of carbonate eluent background conductivity being close to that of hydroxide one. The method is based on the use of carbonate removal device at the optimized conditions which is placed between suppressor and conductivity detector. Background runs 0.2 ~ 0.4 uS/cm with less than 0.1 nS/cm short term noise. With this improved method, various trace analysis applications were made. Trace anions in ultra pure water, halogenated oxy-anions in drinking water, and anionic species in fine atmospheric aerosol, PM-2.5 are among the application examples. Preliminary results for gradient elution will be presented as well.

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An Investigation on the five arsenic species in a seaweed

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목포대학교 화학과 [1]목포대학교 자연대 화학과

Arsenic is well known as a toxic substance, and its toxicity depends on its species. The inorganic arsenic (As^{3+} and As^{5+}) are more toxic than organic arsenic while the arsenobetaine (AsB) and arsenocholine (AsC) have been reported to be nontoxic. Therefore, the importance on research of arsenic species has greatly increased. It is necessary to develop the sample preparation and the analytical method for the determination of arsenic species because the oxidation states of arsenic species should not be converted into each other. In this study, we focused on the matrix interference for the quantitative analysis of arsenic species in a seaweed by ion chromatography (IC) combined with inductively coupled plasma - atomic emission spectroscopy (ICP-AES). Various sample preparation methods were investigated to eliminate the matrix interference. The determination of the five arsenic species in a seaweed was carried out successfully.

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A study on the speciation of vanadium (V^{4+} and V^{5+})

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목포대학교 자연대 화학과 [1]목포대학교 화학과

Toxic and biological effects of vanadium depend on its chemical species in a sample. Of the chemical species of vanaium (from -1 to +5), vanadium(Ⅳ) and vanadium(Ⅴ) mainly exist in the environment, and the vanadium(Ⅴ) is more toxic than the vanadium(Ⅳ). Thus, an accurate determination of each species is typically critical to evaluate the environmental and biological risks. The stability of the vanadium species is affected by its complex state, the pH of the solution, and the matrix in a sample. In this study, we have focused on the development of the analytical method of the vanadium species (V^{4+} and V^{5+}) in a sample by Ion Chromatography (IC) coupled with Inductively Coupled Plasma - Atomic Emission Spectrometer (ICP-AES).

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Glucose deprivation induce alteration of energy metabolism in metastatic cancer cell

이주은 남미소 류도현* 황금숙[1],*

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Tumors show a strong addiction to glucose, which is used and metabolized for cancer cell to produce energy for proliferation and survival. Surprisingly, tumor cells can keep alive although they are exposed to glucose deprivation condition. This means cellular metabolism of cancer can be altered according to their micro-environment. To investigate the effect of glucose restriction on cancer metabolism, integrated metabolomics and transcriptomics approaches were performed. We evaluated metabolic and transcriptomic changes in cell extracts after glucose deprivation. Oxidative phosphorylation was highly up-regulated in metastatic cancer cell exposed to glucose restriction compared to normal glucose condition. Aspartate was highly accumulated in glucose deprived cell through glutamine-driven TCA cycle. This means ATP synthesis was increased and the energy was provided to cancer cell in no glucose condition. Moreover, up-regulation of glutathione-glutamine metabolism allowed cancer cell to reduce oxidative stress from a lack of nutrients and survive despite of extreme condition. These results show the alteration of energy metabolism was a key factor for tumors to survive and integrated approaches are useful tool to investigate biological events in cancer cell.

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Separation and characterization of vesicle by asymmetrical flow field-flow fractionation coupled with multi-angel light scattering (AF4-MALS)

최재영 Emma Magnusson[1] Lars Nilsson[1] Björn Bergenståhl[1] 이승호[*]

한남대학교 화학과 [1]Departement of Food Technology, Engineering and Nutrition, Lund University, Sweden

Vesicles are spherical shell composed of one or several lipid bilayers encapsulating an aqueous space. If there is only one phospholipid bilayer, they are called unilamellar vesicle (ULV), otherwise they are called multilamellar vesicle (MLV). They have been used in many fields, such as model membranes, pharmaceutical and cosmetic industries as nano-scale containers for drugs and other substance.The size distribution and lamellarity of vesicles have been studied by dynamic light scattering (DLS), electron microscopy (TEM or SEM) and nuclear magnetic resonance (NMR). DLS is easy to use and is widely used for the size determination of particles and polymer. Microscopy is useful as it provides informations on both the morphology and the size distribution of the particles at the same time. However, their applications are limited when dealing with complex and/or polydisperse samples.Asymmetrical flow field-flow fractionation (AF4), one family of separation techniques, is useful for the separation and the size characterization of particles in the broad size range from a few nm up to about 100 μm. The objective of this work is to develop a method for the separation and identification of vesicles by AF4-MALS.

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Fluorescence-Raman Endomicroscopic Imaging System for Multiplex Molecular Diagnosis

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Optical-based endoscopic imaging techniques have been intensively explored for use in the diagnosis of specific cancers or for the determination of pathological conditions in suspicious lesions, due to their advantages such as the ability to access specific internal organs, minimal/non-invasiveness, and real-time detection. However, subtle neoplastic changes cannot be clearly identified using only white-light reflectance (WLR) endoscopy in flat and depressed lesions, because conventional WLR endoscopy can offer only visually observable morphological information and not biochemical information from normal or precancerous tissues. For this reason, to improve the accuracy and efficiency of endoscopic diagnosis, many researchers have attempted to combine the additional functionality with endoscopy such as bioluminescence, fluorescence, and Raman scattering.In this study, we designed the real-time fluorescence-Raman endomicroscopic system (FRES) for multiplexed diagnosis with fluorescence-SERS active nanoprobes (F-SERS dots) using optical fiber bundle. In this regard, this system has great advantages for in vivo bio-imaging such as intense signal of fluorescence, high multiplex capacity of Raman scattering, and no-limitation of laser penetration depth. In order to demonstrate possibility of multiplexed detection, synthesized two different kinds of F-SERS dots and their mixture were measured in conical tube. Moreover, for demonstration of in vivo molecular imaging based diagnosis, in vivo and intraoperative targeting in a xenograft tumor model bearing mouse were investigated; these experiments showed that this system can be applied for real-time in vivo molecular diagnosis for cancer during clinical endoscopic examinations

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Investigation of fluorocarbon thin films deposited by inductively coupled and capacitively coupled plasmas

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한국과학기술연구원(KIST) 특성분석센터

Different fluorocarbon thin films were deposited on Si substrates using a plasma-polymerization method. Fluorine-containing hydrophobic thin films were obtained by inductively coupled plasma (ICP) and capacitively coupled plasma (CCP) with a mixture of fluorocarbon precursors C2F6, C3F8, and c-C4F8 and the unsaturated hydrocarbons of C2H2. Process parameters for plasma polymerization such as gas ratio, gas pressure, plasma power, and processing time were investigated. The hydrophobic properties, surface hardness, adhesion strength and wear behavior were elucidated using water contact angle measurements, pencil hardness, 90° peel test, and pin-on-disk wear tester, respectively. The water contact angle measurement showed that the ICP techniques produced more hydrophobic surfaces. Precursors with higher fluorine-to-carbon ratios such as C2F6 have better properties at adhesion ability compared to this result when using C3F8 and c-C4F8.

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Synthesis and Enantioselective Property of on β-Cyclodextrin Capped Zirconia Magnetic Particles

김종화 AVVARU PRAVEEN KUMAR 이용일*

창원대학교 화학과

The separation of chiral compounds is one of the most interesting and challenging tasks because of their identical physical and chemical properties. Magnetic materials possessing chiral functionality on their surface can not only exhibit magnetic properties but also recognize chirality. The present work explores the synthesis of carboxymethyl-β-cyclodextrin capped zirconia magnetic nanoparticles (Fe3O4@ZrO2@CMCD) and their application in selective enantioseparation of amino acids. The Fe3O4@ZrO2@CMCD magnetic nanoparticles (CMCDZMNPs) are characterized by transmission electron microscopy (TEM), X-ray Diffraction (XRD), Fourier transform infrared (FT-IR) spectroscopy, thermogravimetry (TGA), elemental analysis (EA), X-ray photoelectron spectroscopy (XPS) and vibrating Sample magnetometer (VSM). As-synthesized CMCDZMNPs are applied for separation of amino acids and it was proposed that the functional groups at chiral center of the amino acid molecules might interacts with hydroxyl group of CMCD and makes hydrogen bond formation resulted in selective adsorption of enantiomer. Most importantly, the synthesized CMCDZMNPs have shown an excellent magnetic property that reflects in their easy separation from solution.Keywords: Magnetic zirconia nanoparticles, Carboxymethyl-β-cyclodextrin, Enantioseparation, Amino acids.

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L-Cysteine capped CdTe quantum dots : fluorescent Property and its application for biolabeling

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창원대학교 화학과

In this research, L-Cysteine (Cys) capped CdTe quantum dots (CdTe@Cys QDs) were synthesized successfully in aqueous solution. The characterizations of CdTe@Cys were characterized by Fourier transform infrared (FT-IR), photoluminescence (PL), transmission electron microscopy (TEM), confocal microscopy and antibacterial test. We found the optimized condition for preparing CdTe@Cys. The PL spectra were influenced by the of ratio of Cd:Te:Cys, pH value, chemical stability of CdTe@Cys. Moreover, the PL intensity of CdTe@Cys can be reactivated by easy technique through addition of Cys. The PL intensity and storage-time of CdTe@Cys QDs were increased noticeably by capping the cysteine on CdTe QD surface. This addition of cysteine results on the reduced antibacterial effect of CdTe QDs. This was further confirmed through thiazoyl blue tetrazolium bromide (MTT) assays that show the stability of CdTe@Cys in cells as a function of concentration of extra Cys. Antibacterial effect was restrained by adding Cys (> 0.09075 mg/mL) the Likewise, sharp improvement of cell viability reveals the reduction of cytotoxicity(> 5 mg/mL of adding Cys). The images of fluorescence microscope of the CdTe@Cys conjugated to E.coli were observed.

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Quantitative analysis of artificial sweeteners by capillary electrophoresis with a multi-capillary designed molecular imprinted solid phase extractor

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창원대학교 화학과

A novel coupling system of capillary electrophoresis (CE) and monolithic molecular imprinted polymer (MIP) was developed for selective and sensitive determination of sweeteners; sucrose, sucralose, and aspartame, based on an in-column and open-tube molecularly imprinted solid phase extraction (MISPE) concentrator. The MISPE was fabricated by coating a short layer of MIP material (about 3 mm long) directly at the inlet end of the inner wall of a few short capillaries (about 3 cm) under the irradiation of light emitting diode (LED). Two MIP capillaries were connected with CE separation system for analyzing two kinds of sweetners simultaneously. The main advantages of the develped system are the simplicity, the trace analysis at one time to completely different target materials, and the ease of automization. Compared with the conventional method using hydrodynamic injection by MISPE fiber, the MISPE concentrator provides increase in sensitivity without significant loss of separation efficiency.

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Nanoparticle conjugated biosensors for protein biomarkers in conjunction with UV-vis spectrophotometry

백승희 이혜진*

경북대학교 화학과

본 포스터 발표에서는 핵산 기능성을 도입한 금 나노입자를 이용하여 단백질 바이오마커를 UV-vis 분광법으로 간단하게 검출할 수 있는 센싱 플랫폼을 개발한 결과를 나타내었다. 이를 위해 먼저, 모델 바이오마커를 선정하고 이와 특이적 반응성을 가지는 핵산를 고안하여 고안된 핵산의 여분의 DNA 서열에 상보적 결합이 가능한 complementary DNA 를 금속 나노입자로 고정하여 바이오마커/핵산/complementary DNA-금 나노입자 복합체가 형성될 때 바이오마커 농도에 따라 UV-vis 흡광도가 정량적으로 변화하는 결과를 나타내었다.

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Quantitative analysis of cerium in potassium chloride matrix by laser-induced breakdown spectroscopy using a compact diode-pumped solid-state laser

이용훈* 공용득 한송희[1]

목포대학교 화학과 [1]목포해양대학교 교양과정부

Laser Induced Breakdown Spectroscopy (LIBS) with a cmpact diode-pumped solid-state laser (DPSSL) source was applied to analyze cerium (Ce) in potassium chloride (KCl) matrix. The spectral window between 400 and 440 nm was selected for this analysis due to availability of many Ce II and a few Ce III lines along with the K I lines at 404.414 and 404.721 nm that are useful for spectral intensity normalization. Multivariate data analyses using principal component regression (PCR) and partial least squares regression (PLS-R) were performed to calibrate the LIBS spectra to the Ce concentration. The effectiveness of data preprocessing for the multivariate calibrations was discussed. Also, the feasibility of univariate calibration was investigated. Based on the integrated intensities of partially-resolved emission lines, a dependable calibration curve could be obtained. The limit of detection of Ce (0.074 wt.%) was obtained from the univariate calibration curve.

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Comparison of MALDI-based and ESI-based Quantitation Methods for Citrullinated Proteins

신은비 차상원*

한국외국어대학교 화학과

Citrullination is one of the post translational modifications of arginine which results in conversion of arginine into citrulline through deimination and this modification is frequently observed in synovial fluids of rheumatoid arthritis patients. There have been several reports about mass spectrometry (MS)-based detection of citrullinated proteins or peptides via chemical labeling with glyoxal derivatives, but quantitation of citrullinated peptides has been scarcely reported. Recently, Deforce and co-workers reported that citrullination-induced skewed isotope distribution patterns could be used for citrullination quantitation by electrospray (ESI) ionization MS (Journal of Proteome Research, 2012, 11, 5245-5251). In their approach, however, there are some obvious weak points. First, since ESI produces several differently-charged ion species for a given peptide, selecting the appropriate charge state for quantitation is not a routine process. Second, since citrullination causes the loss of the amine group which can be charged, ion production efficiency of noncitrullinated and citrullinated peptides for a given charge state can differ. In this presentation, we investigated whether MALDI possesses the same weakness as ESI in skewed isotope pattern-based quantitation of citrullinated peptides. Our results showed that mono-charged ion species generation in MALDI is beneficial over ESI in citrullinated protein quantitation.

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Graphene Oxide Embedded Thin Sol-Gel Film for Small Molecule Analysis by Laser Desorption/Ionization Mass Spectrometry

이광빈 배상은 허성 차상원*

한국외국어대학교 화학과

Graphene oxide (GO) has been widely used for a matrix of laser desorption/ionization (LDI) mass spectrometry(MS) of small molecules because GO has relatively lower matrix noise than conventional MALDI matrixes such as 2,5-dihydroxybenzoic acid and also because GO effectively ionizes some neutral molecules such as oligosaccharides which are often hard to be ionized by conventional MALDI matrixes. However, use of carbon-based materials is not desirable for time-of-flight (TOF) mass spectrometers since carbon nanomaterials stick to TOF electronics and therefore cause the instability of the MS operation. In order to overcome this issue, we developed GO embedded sol-gel film substrates for LDI MS of small molecules. Our results showed that the GO sol-gel film matrix substrate produced a much lower background noise than the aqueous GO particle matrix. This suggests that ablated carbon materials were significantly reduced when using the sol-gel film substrates. In addition, GO-embedded sol-gel film produced very clear and intense profiles of small metabolites in the region of m/z 100 - 300. Various examples of small molecule analysis with the GO film will be demonstrated in this presentation.

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Further Optimization of Matrix-Assisted Laser Desorption/Ionization for Gangliosides

이동건 차상원*

한국외국어대학교 화학과

Gangliosides, glycosphingolipids with one or more sialic acids, are one of the lipids which undergo severe in-source fragmentation during matrix-assisted laser desorption/ionization (MALDI) process. We previously reported that 5-methoxysalicylic acid (5-MSA) is the very effective matrix for gangliosides since minimal in-source fragmentation of gangliosides was observed with the 5-MSA matrix. In this study, we further investigated the LDI performance of 5-MSA by comparing its property with those of its isomers and several known conventional MALDI matrixes. In addition, we optimized ionization of gangliosides by employing various salt additive conditions. Our results showed that cationization of gangliosides through cesium ions in the positive ion modes have several advantages over other salt additives. First, heavy cesium ions spread mass spectral profiles of gangliosides over wider m/z ranges and therefore reduced spectral complexity. Second, cesium adduct ions gave the better sensitivity than other adduct ions.

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FABRICATION OF GRAPHENE OXIDE THIN FILM DECORATED BY AN FLOWER LIKE TITANIUM DIOXIDE NANOSTRUCTURE APPLYING FOR SERS

TSOGOO ARIUNZAYA 김종화 이용일*

창원대학교 화학과

Graphene oxide (GO) films are semi-transparent films with a few hundred nanometers thick which have recently become commercially available. GO is the oxidized form of graphene which can be visualized as a graphene sheet with its basal plane decorated by oxygen-containing groups. For synthesis of GO, we have selected Hummer's method which is well known for preparing GO from graphite. We report the deposition of films composed of overlapped and stacked plates of GO reduced by a spin coating (SC) method on the fluorine doped tin oxide (FTO) glass. GO thin film surface decorated by our synthesized flower-like titanium dioxide nanostructures (TiO2 NSs). We will discuss the possibility that GO and flower like TiO2 NSs can be used for enhancing Raman signals of adsorbed molecules.

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Morphological Study of Thin Films using Small-Angle Neutron Scattering

신태규

한국원자력 연구원 중성자과학연구부

Small angle neutron scattering (SANS) is a non-destructive and quantitative analysis tool for the investigation of the structures of materials of mesoscopic scale. The scattering signal observed in a typical SANS measurement can be directly related to the informative morphological properties such as shape, size, volume fraction and distribution of particles of the investigated specimen. In this presentation some novel SANS results of solid and organic thin films of ~100nm thickness measured at 18m SANS instrument of HANARO cold neutron facility of Korea Atomic Energy Research Institute, Daejeon, Korea.

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Nonaqueous Capillary Electrophoresis for High Sensitive Simultaneous Detection of Synthetic Organic Dyes

이현호 박문희[1] 방승훈[2] 강성호*

경희대학교 응용화학과 [1]경희대학교 일반대학원/화학과 [2]국방부과학수사연구소 문서지문과

A novel nonaqueous capillary electrophoresis (NACE) method was developed for high sensitive detection of various synthetic organic dyes (i.e., crystal violet, methyl violet B, methyl violet B base, rhodamin 6G, and rhodamin B base) using a laser-induced fluorescence (LIF) detector. Elution behaviors of the dyes in a fused-silica capillary (75 µm I.D. x 365 µm O.D.) were observed in various organic solvents such as methanol, ethanol, dimethylformamide, dimethylsulfoxide, and acetonitrile. The NACE separation optimum condition was 20 mM sodium borate and 870 mM acetic acid in dimethylformamide solvent under the electric fields of 400 V/cm. The dyes were detected within 13 min with excellent baseline separations (resolution ≥2.041). The limits of detection (crystal violet, methyl violet B, methyl violet B base, rhodamin 6G, and rhodamin B base) were 3.40 x 10^{-11} M, 2.94 x 10^{-10} M, 4.33 x 10^{-10} M, 1.11 x 10^{-14} M, and 4.20 x 10^{-16} M, respectively. Enhanced detection sensitivity of the NACE-LIF method should contribute to the high sensitive detection on a trace analysis and forensic science.

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고에너지물질 분해물의 질량분광 연구

배광태 고은미 조수경*

국방과학연구소 국방고등기술원

기존화약에 대한 고성능화 방안으로 분자 내의 질소 함량을 늘리는 연구가 많이 수행되고 있다. 또한 고질소 함유 고에너지물질은 폭발 반응 뒤에도 환경에 유해한 일산화탄소, 이산화탄소 등을 현저하게 적은 양이 생성될 것으로 예측되고 있다. 이들 폭발 분해물을 정확하게 추정하기 위해서는 순간적인 화합물 분석 작업이 매우 중요한 과제이다. 펄스형 질량 분광기는 고에너지물질의 폭발 반응과 분해 메커니즘을 규명하기 위한 중요한 분석장비이다. 본 연구에서는 본 실험에서 신규합성한 고질소 함유 고에너지물질과 기존 화약물질들의 질량분광 결과들을 비교하여 조사 분석작업을 수행하였다.

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Structural and biochemical characterization of APIP as an MtnB enzyme in methionine salvage pathway: a link between cell death and sulfur metabolism

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숭실대학교 화학과

APIP, Apaf-1 interacting protein, has been known to inhibit two main types of programmed cell death:apoptosis and pyroptosis. Seemingly related to this function, APIP was recently found to be associated with cancers and inflammatory diseases. Distinct from its inhibitory role in cell death, APIP was also shown to act as a 5-methylthioribulose-1-phosphate dehydratase (MtnB) in the methionine salvage pathway. Here, we report the structural and enzymatic characterization of APIP as an MtnB enzyme with a *Km* of 9.32 μM and a *Vmax* of 1.39 μmol min^{-1} mg^{-1}. The crystal structure was determined at 2.0 ? resolution, revealing an overall fold similar to members of the zinc-dependent class II aldolase family. APIP/MtnB exists as a tetramer in solution, and exhibits an assembly with *C4* symmetry in the crystal lattice. The pocket-shaped active site harboring a zinc ion is located at the end of a long cleft between two adjacent subunits. We propose an enzymatic reaction mechanism involving Glu139* as a catalytic acid/base, as supported by enzymatic assays of active site mutants, substrate-docking study, and sequence conservation analysis. We explored the relationship between two distinct functions of APIP/MtnB, cell death inhibition and methionine salvage, by measuring the ability of enzymatic mutants to inhibit cell death, and determined that APIP/MtnB functions as a cell death inhibitor independently of its MtnB enzyme activity for apoptosis induced by either hypoxia or etoposide, but dependently for caspase-1-induced pyroptosis. Our results establish the structural and biochemical groundwork for future mechanistic studies of the role of APIP/MtnB in modulating cell death and inflammation, and the development of related diseases.

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A novel N-end rule inhibitor, targeting the Arg/N-end rule pathway

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AbstractThe ubiquitin-proteasome system (UPS) has revolutionized our concept on proteins degradation for a long time, and a subset of UPS, named the N-end rule pathway, which states that the N-terminal amino acid of a protein determines its half-life, has been implicated in various essential cellular processes and human diseases. In eukaryotes, the N-end rule pathway consists of two branches, the Arg/N-end rule pathway and the Ac/N-end rule pathway. The Arg/N-end rule pathway involves N-terminal arginylation while the Ac/N-end rule pathway targets proteins containing N-terminally acetylated residues. However, the physiological functions of both this two N-end rule pathway branches have not been fully understood and the discovery of N-end rule inhibitors has become more important considering its clinical applications. Our research identified a novel Arg/N-end rule pathway inhibitor, it showed significant inhibitory effects on the degradation of Arg/N-end rule substrates not only in vitro and in vivo but also in the mice brains. Moreover, it also inhibited degradation of physiological substrates of the Arg/N-end rule pathway. Taking advantage of in silico docking computational assay, we found that this small-molecule has higher binding affinity with UBR proteins. We anticipate this cell-permeable chemical can be used to understand the pathophysiological processes regulated by the N-end rule pathway.

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Development of a Novel Method to Selectively Degrade Pathological Proteins Implicated in Alzheimer's Disease

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Aggregated or proteotoxic proteins are frequently observed in Alzheimer’s disease (AD) brains which may link to the decreased or impaired proteasomal activities. Herein, surface-modified MSNs as proteasome delivery system show significant advantages on enhancement of proteolytic activities resulting in degradation of tau, proteotoxic protein related on AD. Nickel-charged MSNs were finely synthesized to bind easily to His-tagged 26S proteasomes (≥3MDa) that were affinity-purified from HEK293-pre1-HTBH (His-TEV-Biotin-His) cells. Chemophysical analysis shows that Nickel-charged MSN has enough pore size to contain the proteasome, and surface charge was moderately changed, indicating of non-covalent interaction between proteasomes and MSNs. Biochemical analysis revealed that mega-dalton-sized proteasome complexes can be internalized into the cells through clathrin-mediated endocytosis without cytotoxicity, and still retained proteolytic activities recovered from acidic endosomal condition. Biological assay shows that direct delivery of active proteasomes specifically targeted tau proteins overexpressed and aggregated in cultured cell models without detrimental nonspecific proteolysis. Moreover, ROS-induced cytotoxicity might be inhibited by proteasome delivery. Accordingly, we identified that proteasome delivery using MSNs is beneficial strategy to facilitate degradation of proteotoxic proteins which are implicated in cellular stress or neurodegenerative disorders.

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Preparation of Polyubiquitinated Reporter Substrates for Monitoring Proteasome Activity and Deubiquitinating Activity

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The ubiquitin proteasome system (UPS) is the major cellular mechanism that degrades proteins to short peptides. Most of proteasome substrates are labeled with polyubiquitin chains by E3 ubiquitin ligases for proteasomal degradation. Ubiquitin is activated by the ubiquitin-activating enzyme (E1) and then transferred to ubiquitin-conjugating enzyme (E2). E2 transfers the activated ubiquitin to the protein substrate that is bound specifically to a particular ubiquitin ligase (E3). Repeated conjugation of ubiquitin can generate polyubiquitin chains. These poly ubiquitinated substrates are recognized by the proteasome regulatory particle (RP, 19S) and broken by three kinds of catalytic sites in the core particle (CP, 20S). Here we present a novel reconstitution method to generate polyubiquitinated Sic1 with PY motif, which functions as degradation signal (Ub-Sic1^{PY}) as in vitro proteasome substrate. We affinity-purified recombinant proteins such as E2 enzyme Ubc4, E3 enzyme Rsp5, and Sic^{PY}, which were incubated with the E1 enzyme Uba1 and ATP to induce polyubiquitination. Ub-Sic1 was confirmed by immunoblotting and identified that it was degraded and deubiqutinated by purified 26S proteasomes. These results show that our novel method can be widely used to understand UPS-mediated protein degradation and monitor proteasome activity.

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Increasing Mammalian Proteasome Activity by Gate Opening

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It is now well recognized that accumulation of misfolded proteins is involved in neurodegenerative diseases and various human diseases. It has been demonstrated that effective degradation of proteotoxic protein by increasing proteasome activity. Proteasomes degrade misfolded or damaged protein by proteolysis. The proteasome is the ~2.5 MDa holoenzme complex consisting of two distinguishable the 19-subunit regulatory particle (RP, also known as the 19S) and the 28-subunit core particle (CP, also known as the 20S). CP is a cylindrical complex composed of four stacked rings. The internal two rings are made of seven β-subunits (β1-7) that contain catalytic sites. And the outer two rings are made of seven α-subunits (α1-7). The α-rings function as the "gate" when substrates enter to the barrel. Previous studies demonstrate that the N-terminus of α3 subunit is a key component of "gate". Here we show enhanced proteasome activity through opening the gate by deletion of N-terminal amino residue of a3 (α3∆N), which mainly addressed by using transient overexpression of α3 ∆N-flag diseases or stable cells expressing the mutant form of α3. We observed comparable configuration between the wild-type and α3∆N mutant proteasome from Coomassie brilliant blue staining, silver staining and immunoblotting against CP and RP subunits. Wild type and α3∆N mutant mammalian proteasomes were obtained by using the streptavidin-affinity purification method. Proteolytic activity of the α3∆N proteasome was measured by using fluorogenic short peptides and model substrates such as Ub-sic1^{PY}. These results provide that deletion of α3 N-terminal amino acid residues enhanced proteasome activity and more efficiently degrade proteins which are known to be implicated in neurodegenerative diseases.

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Analysis of *in vitro* ECM Composite Fiber Architecture

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In vivo extracellular matrix (ECM) proteins exist as composite fibers in order to sustain their structure and function. However, current *in vitro* studies have focused on mimicking a single ECM protein fiber. Here, we propose that it is able to recapitulate ECM composite fibers by using glycosaminoglycans (GAGs) mimicking polymer surfaces and analyze their chemical structures by fourier transform infrared spectroscopy (FT-IR) images. At first, polystyrene sulfonate (PSS) was used to provide negatively charged domains to mimic GAGs which are responsible for ECM protein fibrillogenesis through electrostatic interaction and following protein unfolding. Thus, PSS spincoated or patterned surfaces successfully recapitulated both ECM protein single fibers and composite fibers. In order to analyze the fibers, FTIR images were used to show both protein spectrum and images based on specific protein secondary structures. As a result, architecture of divers ECM protein fibers can be chemically mapped by FTIR images without the need to do further treatments for protein imaging.

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Preparing the sterilized nanomateirals for assessing the cytotoxicity of nanomaterials

박수진 정민숙 송미령 김준성*

(주)바이테리얼즈 부설연구소

Currently, nanomaterials are worldwide produced and used in various commercially available applications, as a result, nanotoxicology research is now gaining attention. However, nanomaterials can be contaminated with endotoxin during production or handling. In nanotoxicology studies, contaminated nanomaterials can result in unexpected results.We present an overview of sterilization methods and LAL assay for nanomaterials and focus on limitations of applicaton caused by nanoparticle properties.

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A new small-molecule inhibitor of the CLC-Ka chloride channel and its molecular mechanism of inhibition

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The CLC-Ka and CLC-Kb chloride channels, which belong to the CLC (voltage-gated chloride channel) family, are specifically expressed in kidney and inner ear, where they play a major part in generating osmotic gradient and endolymph production. Mutations in the gene encoding CLC-K channels and barttin, a vital subunit of CLC-K channels, lead to kidney diseases, Bartter syndromes, and deafness. Specific inhibitors could thus have significant values not only for clinical applications but also for investigating molecular mechanisms of CLC-K channels. We have discovered a novel inhibitor, RT-66, which specifically blocks CLC-Ka over CLC-Kb with IC_{50} of 3.2 ± 0.7 μM against CLC-Ka and of 240 ± 45 μM against CLC-Kb. To further elucidate the molecular mechanisms of RT-66 inhibition, we hypothesized that RT-66 would preferentially block CLC-Ka over CLC-Kb through 1) electrostatic repulsions with negatively charged residues on CLC-Kb and/or 2) electrostatic interactions with positively charged residues on CLC-Ka since RT-66 is a negatively charged molecule. To test these hypotheses, we examined RT-66 inhibition against CLC-Kb(D68N) and CLC-Ka(N68D) mutants. CLC-Kb(D68N) exhibited an increased sensitivity to RT-66 while CLC-Ka(N68D) showed a reduced sensitivity. We also investigated a putative role of K165 on CLC-Ka, a major residue of CLC-Ka gating at alkaline pH. We tested RT-66 inhibition against CLC-Ka at pH 10, where half of the lysine residues become neutral; pKa of lysine is around 10. RT-66 blocked CLC-Ka by 34% at pH 10, which is only half of the value obtained at pH 7.4 (63% inhibition), which implies that RT-66 might interact with K165 on CLC-Ka.

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The prediction study of protein-protein interaction residues for the bovine CAPN1/CAST4 system

채한화

농촌진흥청 국립축산과학원/동물유전체과

The HCV-induced CAPN activation and its effects on the virus-infected cell in the host-immune system have been recently studied that the HCV-nonstructural 5A protein plays roles of both an inducer and a substrate for host CAPN protease, participates in suppressing the TNF-α-induced apoptosis response and downstream IFN-induced antiviral processes as well as IFN-resistances. However, any information is not known for disturbance of antiviral responses generated by the bovine CAPN activation by the BVDV, which had been a surrogate model of HCV and is one of the most destructive diseases leading to great economic losses in cattle herds worldwide. This is also thought to be associated with the effects of either small CAPN inhibitors or the natural inhibitor CAST that mainly bind to the binding site of CAPN substrate proteins and competitively inhibit the binding of the enzyme substrates, to possible defensive roles against the two viruses (HCV and BVDV) for anti-viral immunity. For exploiting a new stratagem of discovering lead candidates for anti-BVDV drug, we first attempted to understand the CAPN-CAST interaction sites from bovines and the interaction constraints of local binding architectures and of aqueous-exposed hydrophobic interactions of between the proteins with focused on their impact on protein stability, binding affinity, and aggregation in the bovine CAPN/CAST complex by calculating the mutation energy effects with the corresponding single-point alanine mutations. The observed results suggest that the distinct interaction preferences of the bovine CAPN regulation system are directly related their trace residues; conserved residues, class-specific (the CAPN1 isoform), and species-specific (for bovine) in mammalian CAPN group. The depth and breadth of interaction sites, with CAST concentrated on the distribution of the class- and species-specific residues to detect the CAPN1 specificity, were well reflected to the geometry of between the pharmacophore features and its shape constraints using our modelled CAPN1/CAST complex structures. The CAPN1 specific residues affect the complex stability

(in particular, the hydrophobic interfaces with high spatial aggregation propensity are main factors for the enzyme stability and itself aggregation) rather than its functionality (as binding affinity with Ca+2 ions). The CAPN stability is also correlated with not only to decrease the enzyme itself aggregation but also to increase its small molecular inhibitor efficiency. Conversely, the CAPN conserved residues did influence more its functionality having almost same affinity of the CAST inhibitor and sharing similar Ca+2 ions-binding motifs important for the protease activity in mammalian CAPN group. The two interaction sites (the key residues included in Gln109, Gly113, Lys171, and Trp298 of the first site and Lys578, His579, Trp616, and Arg627 of the second site) with the CAST inhibitor from the bovine CAPN1 were founded to be important for the CAPN inhibition. Surprisingly, the importance of two sites was quite matched with the binding sites of small inhibitor molecules for human CAPN such as α-ketoamide-type inhibitor (ZLAK-3001 and SNJ-1945 in PDB code 2R9C and 2G8J, respectively) and PD150606 (in PDB code 1NX3). Further, we are going to advance computer-aided molecular design of anti-BVDV drug as mimetic CAST inhibitors to develop a rule-based screening function for adjusting the puzzle of relationship between bovine CAPN1 and the BVDV nonstructural proteins from all of the data obtained in the study.

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Imaging of bindings between chemical drug and its target protein kinases by redistribution assay in live cells

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For directly imaging the bindings between chemical drugs and their target protein kinases in live cells using a redistribution assay, we have developed a methodology. Briefly, the HaloTag protein (HT) was fused to Protein kinase C (PKC), which enables the chemical drug and its target protein kinase to cotranslocate from the cytoplasm to the plasma membrane. PKC is well known to translocate from the cytoplasm to the plasma membrane in response to physiological stimuli, as well as exogenous ligands such as phorbol esters. The HT is a mutant of a hydrolase protein that efficiently forms a covalent bond with the HT ligands such as aliphatic halogenated compounds. In particular, we initially modified the chemical drugs (e.g. Dasatinib) with 6-chlorohexyloxyethane. The resulting compounds were cell-membrane permeable, and binding both HT and its target protein kinases. To verify our approach, the fusion construct PKC-mRFP-HT and each of the eGFP-tagged dasatinib target kinases (CSK, SRC, and LYN) were transiently cotransfected into HEK-293T cells and the cells were treated with Halotag Ligand-labelled dasatinib. When the exogenous ligand phorbol 12-myristate 13-acetate (PMA) was added, both PKC fusion and eGFP-tagged dasatinib target kinase were cotranslocated to the plasma membrane. To image the FKBP12-rapamycin-FRB complex, PKC-mRFP-Streptavidin (SA)/eGFP-FRB/TaqBFP-FKBP12 cotransfected cells were pretreated with biotin-labelled rapamycin before PMA treatment. As expected, treatment with rapamycin induced an interaction between FKBP12 and FRB, FKBP12 and FRB were cotranslocated to the plasma membrane.

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A coupling of Proteorhodopsin and Photosystem II; synergetic-regulatory generation of proton gradient in a single vesicle

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The most common uses of electrochemical potentials in living cells are to use for energy storages, which are transferable to various essential cellular activities, i.e. the generation of ATP or NADPH, and ions or molecular transport across a membranes. The electrochemical potentials are produced by activation of light-harvesting membrane proteins. Depending on the cells from various species, different membrane protein complexes are acting similar roles, in terms of generating an electrochemical potential, by absorbing different light-spectrum. For example, proteorhodopsin (PR) and photosystem II (PSII) are well-known photoactive transmembrane proteins, functioning as a light-driven proton pump in marine planktonic bacteria, archaea, and eukaryotes and splitting of water in thylakoid membrane of plants, algae, and cyanobacteria, respectively. Although their light-driven mechanisms and their utilizing wavelength bands are very much different, both systems can result a similar proton gradient across the lipid membrane. By reconstitution of two different purified proteins into a single giant unilamellar vesicle, we could successfully build the hybrid light-harvesting liposomes incorporated both with PR and PS II, activated by the wide wavelength bands, from blue up to red. This new system, generating improved gradients of electrochemical potential across a membrane. Furthermore, according to dependent absorption of membrane proteins, we could control activation of membrane proteins by using different wavelength to regulate internal pH. This new system can be used as numerous energy storages in vitro, providing photo-induced energies for flagella rotation, NADPH synthesis or ATP synthesis with highly improved light efficiencies.

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Detection of Non-Coding Cellular RNA by Force-based Mapping

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MicroRNA (miRNA) is a class of short (19-25 nt) noncoding single strand RNA as a regulator on target transcript in post-transcription. miRNAs have important roles in multiple biological functions such as cell differentiation, proliferation, and apoptosis. Additionally, the expression level of miRNAs is associated with various human diseases. Thus, miRNA detection has become an important emerging topic in biomedical fields. For the accurate analysis of miRNA, it is necessary to discriminate pre-miRNA from miRNA because of sequence similarity between miRNA and pre-miRNA. In this study, we focused on the discrimination to quantify the accurate distribution of our target molecule on the substrate. We optimized the condition for discriminative hybridization between these RNAs to discourage the binding of pre-miRNA on the capture probe spotted substrate by controlling the factors affecting the denaturation of pre-miRNA. We generated specific force maps to visualize the detection of RNA/DNA hybrids onto substrates by atomic force spectroscopy (AFM). We examined whether an identical tip tethering the RNA/DNA duplex detectable bio-molecule would be able to discriminate between these RNAs. We also proved the influence of the hybrid structure on the force-based detection. Consequently, we found that force-based mapping would show the quantitative distribution of target molecule and we also expect this AFM-based study will lead us to development of an ultrasensitive miRNA detection tool.

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Imaging of Non-coding Cellular RNA in a Tissue Using Atomic Force Microscopy

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MicroRNAs (miRNAs) is a class of small (19-25 nt) non-coding RNA molecules which regulates in post-transcriptional gene expression. miRNAs have multiple biological functions such as cell differentiation, proliferation and secretion. Especially, specific miRNAs of brain have important roles in neuronal differentiation, development, plasticity and induced neurological disorders. Distribution of miRNAs have become an important emerging topic in biomedical fields. Therefore, spatial distribution of miRNAs is important to the single neuron, because the expression level of miRNAs is differentially associated with neuronal region such as soma, dendrite, axon, and synapse. miRNA-dependent fine-tuning has regulated various biological functions and induced diseases, but the distribution of miRNAs is not well reported.Conventional methods widely used in the detection of miRNAs mainly include northern blotting, microarray, real-time RT-PCR and in-situ hybridization. However, conventional tools are not easy to detect high spatial localization and resolution of miRNAs. Therefore, a new approach for miRNA detection tool is AFM. AFM has become a powerful tool in bio-imaging field, because AFM is possible to measure simultaneously imaging and mapping of interaction forces.In this research, the spatial distribution of a specific miRNA on a sectioned brain tissue is measured by force-based AFM and help to understand functions of miRNA in depth.

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DNA ligase mediated Ag+ ion sensor

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공주대학교 화학과

A novel and highly sensitive two step strategy was designed to detect Ag+ ions in aqueous solution using DNA oligomers and thermostable Tfi DNA ligase. First step involves enzymatic ligation in which silver ions were detected and second step was amplification of the ligated template by RT-PCR. The rate of DNA amplification by RT-PCR can be directly correlated to the amount of silver ions in the ligation reaction. In this system, three oligonucleotides were used for DNA ligation. One is a template DNA for ligation, and the other two oligomers were a full matched sequence DNA and a mismatched DNA oligomer to the template. This strategy makes a way to extend the enzymatic alphabet for the detection of metal ions. The detection limit of silver ions in this method was 1.5 pmol in the ligation reaction.

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Single Vesicle Content Mixing Assay using Novel Host-Guest Binding FRET Pair

공보경 N. Selvapalam 고영호[1] 이남기[2,*] 김기문[*]

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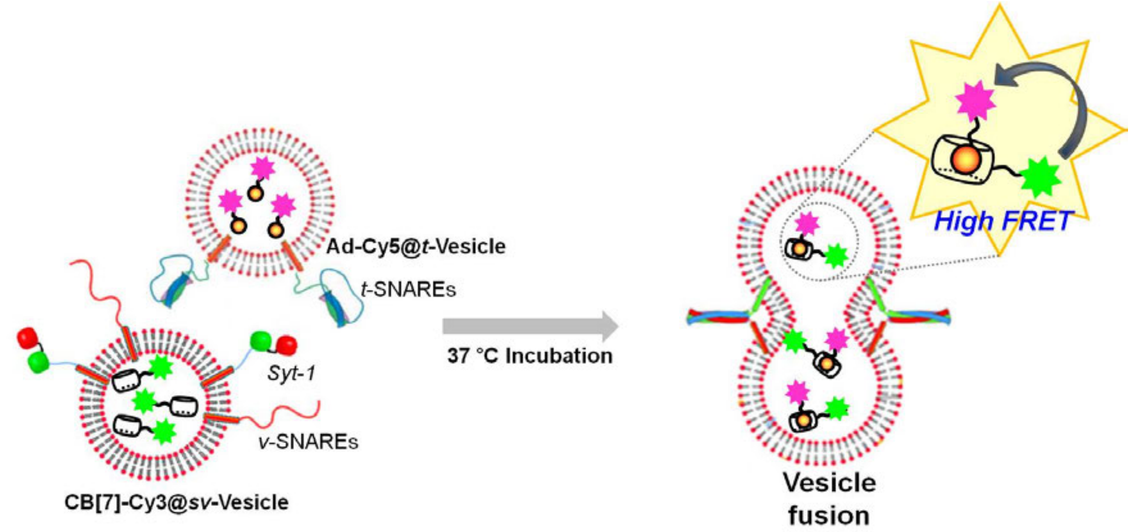
Understanding the molecular mechanism of synaptic vesicle fusion triggered by a conserved family of proteins called SNAREs (N-ethylmaleimide-sensitive factor attachment protein receptors) is a key issue in neuronal communication. In order to study the protein-mediated vesicle fusion mechanism, we designed a synthetic system to observe the synaptic vesicle fusion events at the single-molecular level with the course of time. A SNARE protein based single-vesicle fusion assay monitored by fluorescence enables simultaneous measurement of vesicle fusion. Here, we report a new, reliable and efficient single-vesicle content mixing assay for a SNARE-mediated membrane fusion using a fluorophore (Cy3, Cy5) tagged host-guest pair cucurbit[7]uril?adamentane derivative (CB[7]-Ad), on the basis of fluorescence resonance energy transfer (FRET) analysis. A change in FRET signal occured when a CB[7]-Cy3 binds to a Ad-Cy5, which is a mark of two different SNARE embedded vesicle (CB[7]-Cy3@sv-Vesicle, Ad-Cy3@t-Vesicle) fusion. This synthetic host-guest system may be useful to monitor the vesicle fusion events in detail. Results from this study and their implication in synaptic vesicle fusion will be presented.


Ad-Cy5@*t*-Vesicle
t-SNAREs
Syt-1
v-SNAREs
CB[7]-Cy3@*sv*-Vesicle
37 °C Incubation
High FRET
Vesicle fusion

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Scopoletin induces autophagy via modulation of p53 and histone deacetylases in IMR 90 cells

이수경 김문무 오영희*

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The recent evidences indicate that autophagy is associated with a num ber of processes including aging, muscular disorder and neurodegeneration in addition to longevity. The efficacy of scopoletin was investigated on induction of autophagy through histone deacetylation and p53 activation in human lung fibroblast cell line, IMR 90. In this study, it was discovered that scopoletin induced autophagy. It was also identified that the activation of p53 by scopoletin are related to the induction of autophagy. Furthermore, scopoletin modulates the expression of proteins related to autophagy. The expression levels of p-p53 and Ac-p53 were decreased in the presence of scopoletin. In contrast, the expression levels of histone deacetylase 1 (HDAC1) and sirtuin 1 (SIRT1) were increased in IMR 90 cells treated with scopoletin. In addition, the expression level of SIRT6 was increased in the presence of scopoletin. In contrast, both the expression levels and activity of histone acetyltransferase (HAT) were decreased by scopoletin treatment. Moreover, the level of SA-β-Gal staining, an aging marker, was reduced by treatment with scopoletin. These results suggest that scopoletin promotes the induction of autophagy in IMR 90 cells through inactivation of p53 by the enhanced expression of histone deacetylases related to aging. Therefore, these findings suggest that scopoletin may be a candidate capable of influencing aging related to autophagy.

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Utilizing the Bioorthogonal Base-Pairing System of L-DNA to Design Ideal DNA Nanocarriers for Enhanced Delivery of Nucleic Acid Cargos

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DNA nanoconstructs are a potential drug carrier with high biocompatibility. They are promising particularly when therapeutic nucleic acids are the cargos to be delivered, since both the carrier and the cargo are nucleic acids which can be designed, synthesized and assembled in a seamless feature without using post-synthetic conjugation chemistry. However, the unwanted base-paring events between the cargo and the carrier may potentially disturb the desired structure of the cargo-loaded carrier. To address this concern, we propose a DNA nanocarrier composed of L-DNA strands having a bioorthogonal base-paring system. The study presented here provides useful properties of L-DNA as a backbone for the DNA nanocarrier and demonstrates superiority of L-DNA over the natural D-DNA backbone in the delivery of an anti-proliferative aptamer as well as in the construction of the cargo-carrier assembly.

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Analysis of Interhelical Hydrogen bonds in Transmembrane Helices

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The interhelical hydrogen bonds stabilize transmembrane (TM) helical conformation of integral memebrane proteins and play a pivotal role in folding process. We statistically analyzed characteristics and patterns of interhelical hydrogen bond network in TM helices with known 3D structures of the TM proteins. The dataset of TM protein structures where the transmembrane regions consist of the alpha-helices is made up of the PDBTM database. The non-redundant set of 407 TM proteins was constructed, after removing the proteins with more than 90% sequence identity. The final dataset was made of 240 proteins whose refined 3D structures are available in the PDB_redo database among 407 proteins. The hydrogen atoms were added by using the what_if program. The interhelical hydrogen bonds were identified by using the HBplus program with the default value such as donor-acceptor distance < 3.9Å, donor-hydrogen-acceptor angle > 90°. First, the composition of the 20 amino acids in TM helices was analyzed. We identified the fraction of the polar residues within TM helicse that participate in interhelical hydrogen bonds, any conserved sequence patterns, and dominant polar residues in TM regions. We also confirmed whether polar residues engage ine hydrogen bonds or not and figured out the roles of non-engaged TM polar residues. Lastly, we investigate whether the polar residues forming the interhelical hydrogen bonds play roles of the donors or acceptors and whether these hydrogen bonds are between the side chain and main chain or between the side chain and side chain.The average length and angle of a hydrogen bond was computed. All the features were also evaluated for each TM subsets with the same number of TM segments to find out any characteristics depending on the helical topology.

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Identification of effective ssDNA probes for discrimination between influenza virus subtype H1 and H5

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In the influenza virus infection pathway, the viral surface protein hemagglutinin identifies receptor sialic acid residues present on the host cell surface. It makes hemagglutinin suitable for target to detect the influenza virus. In this study, we constructed hemagglutinin expression vectors and purified the GST-tagged HA1 proteins. Using a Counter-SELEX procedure, we found four ssDNA aptamers, which have specific affinity for the HA1(H1N1). Selected aptaers were shown the dissociation constant of about 100nM that confirmed using SPR and ELISA. The interaction of selected aptamer, purified HA1 and sialic acid on HEK 293T cell were investigated by using laser scanning confocal microscopy (LSCM) and fluorescence-activated cell sorting (FACS). Our selected aptamer have high affinity to H1 subtype and we hope these aptamers would have wide applications in diagnosis, therapy and prevention of influenza virus.

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A ssDNA aptamer prevents influenza infection by blocking the Non-structural 1 protein

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Influenza is an infectious disease caused by RNA viruses of the family Orthomyxoviridae, the influenza viruses. Influenza A virus contains 8 segments of (-) ssRNA that encode 11 known proteins. NS1 protein was known for disrupting the induction of IFNs by first inhibiting the intracellular sensor RIG-I. Therefore, inhibition of NS1 may limit further viral infection in the host cells by activation of IFN induction. Using a SELEX (systematic evolution of ligand by exponential enrichment) procedure, we selected a high-affinity DNA aptamer capable of binding to NS1 protein with a dissociation constant of 18.91 nM. We were measured binding affinity of NS1 protein and aptamer by ELISA and SPR. The aptamer was incubated with 293T cells expressing NS1 and binding assessed by FACS and Confocal. We revealed that the selected aptamer was successfully able to induce IFN and block the viral replication. The aptamer that was isolated in this study are expected to be new molecular drug candidate.

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A New Strategy for Detection of Organophosphorus Pesticides using Enhanced Green Fluorescent Protein and Aggregation-Induced Gold Nanoparticles

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Organophosphorus chemicals (OPs) are primarily used as pesticides and germicides in agriculture. Because the large amounts of OP residues have the toxic substances, and thus make an impact on the environment and humans. It is essential to develop a new strategy for detection of OP residues from agricultural products. The strategy should be simple, convenient, sensitive, and particularly fast on-site than the traditional detection method. Gold nanoparticles (AuNPs) are one of the most extensively used nanomaterials in a biosensor field due to significant colorimetric assay solution and UV/vis spectrum changes caused by the aggregation of AuNPs. Citrate-stabilized AuNPs was synthesized with a size of 13 nm in diameter; a red color and absorbance peak at 518 nm. Enhanced green fluorescent protein (EGFP) emits fluorescence at 508 nm by excitation at 450 nm. It was observed that EGFP had influenced by various kinds of OPs as well as could induce very significant AuNPs aggregation. When AuNPs and OPs were first mixed, the color of the mixture remained to be red. EGFP was subsequently added to AuNPs containing OPs, and the color of AuNPs changed from red to blue or purple immediately and red-shift to 660-670 nm in absorption maximum. This assay is quite sensitive; OPs could cause a clear solution for color change even at a low concentration. Furthermore, this assay does not require complicated sample treatment. Thus, the new strategy could be suggested the fast on-site analysis of OP residues.

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Early diagnosis of tuberculosis using MPB 70 antigen/antibody sandwich complex with quantum dots

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Tuberculosis (TB) is a fatal, infectious disease caused by Mycobacteria. TB commonly attacks the lungs and occasionally affects other parts of the body. However, treatment against TB is difficult and requires administration over a long period of time. Thus, an ideal detection method is required to prevent TB spreading. Mycobacterial protein bovis 70 (MPB 70) is one of the most studied mycobacterial antigens and a major soluble secreted antigen highly expressed by Mycobacterium bovis and M. tuberculosis. Using MPB 70 antigen with two different types of anti-MPB 70 antibodies, we applied a biosensor based on sandwich assay with quantum dots (QDs). QDs are one of the most useful and powerful tools in sensors, because that has a unique property such as emit strong fluorescence, size-tunable, and easy to ligand exchange. QDs were conjugated with one of MPB 70 antibodies by coupling agent (EDC/NHS), and then antibody, antigen and the conjugates were applied to ELISA utilizing polystyrene plate. As a result, a rapid detection method was successfully developed for early diagnosis of TB.

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In Vivo Synthesis of Europium Selenide Nanoparticles and their Biomedical Applications

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중앙대학교 화학과

Last few years, diverse nano-scale metal particles have been synthesized for biomedical applications, which have been used as high-density magnetic storage materials, next-generation display materials, drug delivery system and biomedical materials. To synthesize metal nanoparticles (NPs) used in so many areas, we have used several recombinant proteins. We report diverse metal NPs by recombinant bacterial cells expressing heavy-metal binding proteins, phytochelatin synthase and/or metallothionein. These recombinant proteins have a high affinity to metal NPs which are synthesized within cells using these attributes. However, a limitation of the biogenic NPs is the shortage of control over the particle size. Heterogeneous NPs are mainly produced, which may be derived from the different reaction conditions, such as the concentration of the metal ions surrounding each cell. Furthermore, toxic effect of EuSe NPs for prokaryotes and eukaryotes were in progress. Various metal NPs demonstrate unique optical, electronic, and magnetic properties, respectively, which depend on their composition, size and structure, and have been explored extensively for various applications in bio- and nano-technologies. Herein, we synthesized EuSe NPs, and then its magnetic and optical properties were analyzed. In order to understand in our research, we describe to make it easy and tunable.

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DNA-Conjugated Au-Fe_3O_4 Nanoparticles for Ultrasensitive Monitoring and DNA Separation

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Highly sensitive and selective DNA detection plays a central role in many fields of research including human health, forensic science, and bioanalytical chemistry. Among them, monitoring of DNA in marine organisms has become an increasingly important tool for the detection of marine pollution and seafood safety. Therefore, this work is to provide simple, sensitive, and inexpensive strategy for the DNA detection based on the optical properties of Au-Fe_3O_4 nanoparticles which were prepared by reducing $HAuCl_4$ on the surface of Fe_3O_4 nanoparticles. Synthesized Au-Fe_3O_4 nanoparticles were then hybridized with probe DNA and cysteamine. UV/visible absorption spectroscopy intensity and transmission electron microscopy images show that the quantity and surfaces of Au-Fe_3O_4 nanoparticles. Furthermore, generated color signals of Au-Fe_3O_4 nanoparticles were confirmed with naked eyes. After the reaction with target DNA, Au-Fe_3O_4 NPs were employed to facilitate sample separation utilizing an external magnetic field. Agarose gel electrophoresis was performed for discrimination between target DNA and other DNA. The ease of operation and good separation efficiency has shown an effective potential application using magnetic Au-Fe_3O_4 nanoparticles for DNA monitoring of seafood safety and marine pollution accidents.

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Improve Efficiency and Specificity of PCR Using Carbonized Polydopamine-Coated Silica Nanoparticles

서지민 박태정*

중앙대학교 화학과

Polymerase chain reaction (PCR) can generate a large number of copies of target DNA. It can be used not only as an in vitro DNA amplification method but also used in many bioassay applications. Recently, nanomaterial-assisted PCR for enhancing efficiency and specificity has been investigated such as graphene. Because yield of PCR acts as one of the important factors, optimization of PCR with nanomaterial is essential to perform successful research for better effectiveness. Based on a similar structure with graphene, we choose carbonized polydopamine-coated silica nanoparticle (C-PD SNP) on PCR. This study demonstrated for the first time that C-PD SNP could significantly improve PCR efficiency and specificity. Furthermore, C-PD SNP would be suggested that advantage will apply to capture the other proteins on PCR and other bioassay applications as well.In this paper, we confirmed that best concentration of C-PD SNP, optimal shorter cycle numbers for comparison, and annealing temperature. We used novel materials including C-PD SNP, silica nanoparticle (SNP), polydopamine-coated silica nanoparticle (PD SNP) and graphene oxide (GO) for comparison among them, respectively.

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Genetically Encodable Enzymatic Flavinylation in Living Mammalian Cells

강명균 이현우*

울산과학기술대학교(UNIST) 화학과

Flavins (FMN, FAD and riboflavin) are important cofactors for mediating many redox reactions in living organisms. Interestingly, in nature, there are some proteins are bound to flavin covalently through autocatalytic process and non-autocatalytic process. Inspired from these natural enzymatic labeling system, we could successfully develop the genetically-encodable system to label protein of interest selectively with endogenous flavin in living cell. This system is useful for some application such as fluorescent imaging of target protein and biochemical assay of topology mapping of some membrane proteins.

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Genetically Encodable Peudo-Enzymatic System for Mapping Protein-Protein Interactome in Living Cell

이송이 이현우*

울산과학기술대학교(UNIST) 화학과

Protein is a one of the key functional molecules in our body. In human cell, ~18,000 different kinds of proteins are expressed. Most of these proteins work with other proteins through protein-protein interaction or interactome to make functional macromolecular complex. Therefore, it is very important to understand protein functions in context of protein-protein interaction. However, not many methods for mapping endogenous protein interactome in living cell are developed. In this session, we will show a new protein-protein interaction mapping method using genetically encoded pseudo-enzymatic reaction on the target protein of interest in living cell.

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Peptide Nucleic Acids (PNAs) are an Additional Class of Aptamers

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경희대학교 화학과

Peptide nucleic acids (PNAs) have been known for their similar or superior properties to DNA or RNA since 1991, but not regarded as a separate class of aptamers. We report here an interesting additional property of PNAs revealed by graphene oxide (GO)-based assays, suggesting that nucleobases in certain aptamers play more important roles in strong and selective binding to the target molecules.

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Combination of Aptamer-Functionalized Quantum Dots and Electrophoretic Mobility Shift Assay for Specific Detection and Quantitation of Proteins of Interest

조예슬 이은정 하상수*

경희대학교 화학과

Quantum dots (QDs) are semiconducting nanoparticles with interesting optical properties. The outstanding fluorescent properties of QDs including photostability, high quantum yield, narrow emission bands, broad excitation spectra, and accessibility to versatile functionalization are one of the key advantages for their sensing applications. In the present study, we report QD-functionalized aptamers for specific detection and quantitation of proteins of interest, based on electrophoretic mobility shift assay (EMSA). Among the wide variety of potential biofunctional groups, we used the highly selective interaction between aptamers and oligohistidine or human chorionic gonadotropin (hCG), and the results demonstrate that the combination of the QD-functionalized aptamers and EMSA can be one of the best sensing options for protein quantitation with low limit of detection. In principle, multiplex detection for several proteins on a single gel can be achieved by our method, leading to facilitation and simplification of the routinely used protein detection procedure.

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α-Asarone with Antioxidant Activates Angiogenesis by Modulation of Matrix Metalloproteinase

박혜정 김문무 오영희*

동의대학교 화학과

Angiogenesis is essential component of wound healing, regeneration but cancer cell strongly needs to angiogenesis to receive various nutritive during cancer metastasis. Therefore balancing levels of angiogenesis is very important. Purpose of this study is to investrigate effect of α-asarone on angiogenesis and antioxidant. α-Asarone is a main component of *Acorus gramineus* widely known as a oriental traditional medicinal stuff. Acorus gramineus has been known to have a variety of medicinal effects such as anti-gastric ulcer, antiallergic activity, inhibition of histamine release and antioxidant effect. However, the mechanism of its action remains unclear in human. In this study, the effect of α-asarone on matrix metalloproteinase, antioxidant effect and angiogenesis in cell free system was examined in HT1080 cells. The effect of α-asarone on cell viability using MTT assay showed no cytotoxicity below 16 μM. It was observed that α-asarone exhibited reducing power in addition to protect effect of DNA oxidation. Furthermore, α-asarone increased the expression levels of MMP-2, and -9 stimulated by phenazine methosulfate (PMS) and phorbol 12-myristate 13-acetate (PMA). Especially the expression levels of antioxidant enzymes such as SOD-1 and glutathione reductase was increased in the presence of α-asarone. Furthermore, we found that α-asarone induces angiogenesis through tube formation assay and aorta ring assay. Therefore, above findings suggest that α-asarone may be a candidate for prevention and treatment of pathological diseases by antioxidant, MMP-2, -9 activation and induce of angiogenesis

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The Mechanical Properties of ECM Coated Lipid Vesicles

백시연 신관우[1,*]

서강대학교 화학과 [1]서강대학교 화학과 및 바이오융합과정

It is important to understand the mechanical properties of cell membrane because it’s not only the boundary of the cell that maintain its structure but is involved in many biological processes like apoptosis. We’ve been studying artificial cell, made of phospholipids bilayer, called a lipid vesicle, to mimic the real complicated cell. Recently, we succeed in coating liposomes with collagens, the most abundant protein in the extracellular matrix (ECM), which makes artificial cell more like a real one. To measure the mechanical properties of liposomes, we set up micropipette aspiration that makes it possible to capture single vesicle, apply pressure gradually, and monitor the area expansion of it. With this apparatus, we tried measuring the elastic modulus of ECM protein coated lipid vesicles and compared it with that of pure lipid ones. Then, we could find out how ECM proteins affect the characteristics of lipid bilayer and have more knowledge about the cell.

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In vitro crystallization of lysozyme in a giant unilamellar vesicle as a cellular barrier like plasma membrane

문태우 신관우[1,*] 권오선[*]

서강대학교 화학과 [1]서강대학교 화학과 및 바이오융합과정

Currently one of challenging issues in the interfacial bioscience is how to mimic in vitro the fundamental functions of a living cell with cell structures constructed artificially. Because most cellular functions are related to the structures of proteins, we have studied the features of process of crystallization of lysozyme protein in vitro cellular environment, especially focusing on in vivo the crowding effect in the plasma membrane which encloses a living cell and so acts like a selective permeable barrier between exterior and interior of the cell, are important because it is related to almost all of cellular processes. In order to mimic the different distribution of crystalized proteins in vicinity of the artificial cell membrane, we followed two subsequent steps: (a) Preparation of the giant unilamellar vesicles by coating lipid bilayer on the inside wall of a vial filled with lysozyme solution by the gentle hydration, and (b) Crystallization of lysozyme either interior and exterior of the GUVs by using the hanging-drop method. To investigate the crowding effect various polymers such as agarose gel, PEG, and dextran were mixed followed by the step (a), as a parameter which generates the hydrogel-state in the solution. In order to determine the fundamental properties of gel network, we measured the viscosity and gel formation as a function of the concentration. The more detail analyzing data will be left in future work.

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The way to control enantiopreference and enantioselectivity by BCL-catalyzed hydrolysis of γ-butyrolactone

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한국외국어대학교 화학과

Among many lipases only Burkholderia cepacia Lipase (BCL) shows high enantioselectivity toward chiral primary alcohols, but the molecular features that determine enantioselectivity are unknown. Some stereoisomers of butyrolactones what we used can be an ideal case for explaining and overcoming unpredictability of primary alcohol with lipase-catalyzed hydrolysis. For this purpose, we focus on polar portion in the substrate or enzyme by experiment and molecular modeling. Changing of polar portion of the substrate or BCL shows a chance to control enantioselectivity. With quantitative measurement of correlation between measured enantioselectivity and predicted enantioselectivity, we include umbrella-like inversion which is a new paradigm for binding orientation not only enantiomers but until diastereomers involving reversed enantiopreference. This expansion can brighten primary alcohols in the shade of the purpose of asymmetric synthesis. We suggest to design better substrate to increase enantioselectivity and to change enantiopreference in lipase-catalyzed reaction, which is the way to substrate-engineering in enzyme chemistry.

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Heterodimer formation of human sweet taste receptor T1R2/T1R3

장진철 조현주 이성준 공광훈*

중앙대학교 화학과

Among five human sensory systems, taste sensory system is involved in determination or selection of foods, thus promoting to intake nutrients or to avoid toxins. Especially sweet taste might have helped us to identify carbohydrate-rich food and to ensure energy intake. The perception of sweet taste is induced by the interaction of sweeteners with specific chemosensory receptor which is a heterodimeric receptor composed of T1R2 and T1R3 subunits existing in taste cells. T1R receptors belong to the class C G-Protein Coupled Receptor(GPCR) family that can be characterized by 3 different domains: A large extracellular N-terminal domain(NTD) which provides the primary ligand binding site, cysteine-rich domain(CRD), and hepta-helical transmembrane domain. However, little is known about the exact structure of the human sweet taste receptor T1R2/T1R3 that is critical for the research on sweet taste signal transduction pathway. This dearth of understanding is due in part to difficulties in preparing functional receptors in heterodimeric form. In our study, we separately expressed recombinant human taste receptor subunits without transmembrane domain in Escherichia coli using two different vectors, pGEX-KG for T1R2 subunit and pET-26b(+) for T1R3 subunit. Using affinity chromatography, GST column for T1R2 and His-tag column for T1R3, each subunits were successfully purified. Then, we mixed and reacted subunits in buffer solution to let them stick together automatically as hydrogen bonding is the key for subunit's association. Finally, by using gel filtration chromatography, we formed heterodimeric human sweet taste receptor T1R2/T1R3. These receptors can be used not only for structural determination but also for the study of human sweet taste signal transduction pathway.

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Lipid Flip-Flop in Asymmetric Bilayers - X-ray and Neutron Reflectivity Study

Phan Dinh Minh 신관우[1,*]

서강대학교 화학과 [1]서강대학교 화학과 및 바이오융합과정

The transbilayer movement of phospholipids in cellular membranes, also known as lipid flip-flop or translocation, is an area of significant biological importance. It has long been believed that the translocation of lipids between the inner and outer leaflets of cellular membranes could only occur by a protein-mediated process. However, cells also use passive transport mechanism that facilitates the migration of lipids from one leaflet to the other without proteins. In this study, we aim at the mechanism of lipid flip-flop phenomenon observed by Neutron reflectivity at molecular level. We would like to investigate the effect of charge lipids and unsaturated lipids, which regulate many biological functions and are strongly related to the specific structure of bilayer membrane, 1) whether they cause the lipid disorder to facilitate the flip-flop, 2) how the negative charge is managed to move across the hydrophobic region in the intermediate structure. Solid supported bilayers were prepared using the Langmuir-Blodgett/Langmuir-Schaeffer deposition method and were characterized by X-ray reflectivity obtain the information of bilayer quality.

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Aptamer-and FRET-Based Competitive Binding Assay for Quantitation of Hepatitis B Surface Antigen

서승관 하상수*

경희대학교 화학과

An aptamer-and FRET-based Competitive binding assay for specific target quantitation has been developed. This method has been successfully employed for the fast and sensitive detection of hepatitis B virus surface antigen (HBsAg). Key features of our method include its low intrinsic background noise, low costs, high resolution, and high sensitivity, enabling detection of as low as 1.25 mIU/㎖ without the tedious extraction and/or washing procedures. This assay has better recovery and accuracy than that of conventional competitive binding assay or others for HBsAg quantitation.

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Whitening Effect and Antioxidant Activity of *Ulmus macrocarpa* Ethanolic Extracts in B16F1

권은정 박혜정 이수경 김문무 오영희*

동의대학교 화학과

Melanin plays a key role in protection of skin from ultraviolet that produces generation of reactive oxygen species (ROS). However, the ROS leading to oxidation of lipid, protein and DNA are involved in overproduction of melanin that was known to cause melasma, age spot and freckle. Among herb medicine stuffs used in this study, *Ulmus macrocarpa* was reported to flavonoid. The aim of this study is to investigate whitening and antioxidant effects of *Ulmus macrocarpa* extracts (UMEE) in B16F1 cells. UMEE not only exhibit high reducing power and scavenging activity on DPPH but also inhibitory effect on melanin synthesis. Moreover, UMEE influences the expression of superoxide dismutase-1 (SOD-1) and tyrosinase related protein-1 (TRP-1). These results indicate that UMEE has whitening effect and antioxidant effect, suggesting that it is available for development of whitening cosmetics.

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Engineered split-intein mediated protein trans-splicing reaction and cross reactivities

전용권 권영은*

동국대학교 의생명공학과

Protein trans-splicing reaction (PTS) is self-processing enzymatic reaction mediated by a pair of split-inteins. PTS based protein semi-synthesis enables the introduction of various synthetic probes to target proteins in vivo and in vitro. While the PTS became a useful tool for various biological studies, the difficulties associated with the synthesis of 40mer peptide became a drawback in its applications. Here we have generated several engineered split-inteins by shifting the split-site of naturally split-inteins to new positions. We utilized Npu DnaE intein as a model system as this naturally split-intein mediates fast (t1/2 ~ 1 min) PTS in physiological conditions. In order to investigate how the lengths of N and C intein affect the PTS kinetics, we prepared multiple pairs of split-inteins that consist of various lengths of N and C-inteins. The kinetics of reaction between each engineered pairs and the cross-reactivities were studied.

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The effect of extein pI values in protein trans-splicing reaction

전용권 권영은*

동국대학교 의생명공학과

Protein trans-splicing reaction (PTS) is self-processing enzymatic reaction mediated by a pair of split-inteins. PTS based protein semi-synthesis enables the introduction of various synthetic probes to target proteins in vivo and in vitro. As the PTS became a useful tool for various biological studies, it is important to understand the factors that affect the kinetics of the PTS. For this study, we have chosen Npu DnaE intein as a model system as this naturally split-intein mediates fast (t1/2 ~ 1 min) PTS in physiological conditions. In order to investigate the effect of extein pI's on the PTS kinetics, we prepared multiple pairs of split-inteins that carry exteins of various pI's. We observed accelerated reaction rates as the pI's of N exteins increase. In case of various C intein pairs, we observed accelerated reaction rates as the pI's of C intein flanking sequence decrease. This result provides a good guideline in designing efficient PTS.

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Cell surface anchored neurotrophic factor and their effects

김다희 권영은*

동국대학교 의생명공학과

With the brain's limited capacity for repair, cell transplantation is demonstrated to be an effective therapy for central nervous system (CNS) disorder. While cell transplantation for a number of neural disease have been demonstrated, transplanted cell often exhibit poor viability due to the exposure to hypoxia-ischemia. So the technical advances to improve grafted-cell survival are essential to improve the efficacy of cell transplantation. We are developing an assay tool to screen the effect of various factors to the viability of grafted-cell. In this study, we are utilizing split-intein mediated protein trans-splicing reaction (PTS) to conjugate various proteins to the surface of live cells via covalent interaction. Through this approach, Glial cell line-derived neurotrophic factor (GDNF), which potently promotes the survival of many types of neurons, is anchored to the surface of human neural stem cell. We investigate effects membrane-anchored GDNF on the viability of NSC in effects on oxygen-glucose deprivation (OGD) by using MTT assay. This work suggests a method to maintain high effective concentrations of neurotrophic factors on NSC and can be utilized for enhanced cell-based therapies.

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Examination and application of Ni-NTA-coated microplate for a high-throughput O-GlcNAc transferase's enzymatic activity assay

김은주

대구대학교 과학교육학부/화학교육과

O-GlcNAc transferase (OGT) transfers GlcNAc moiety from UDP-GlcNAc to the hydroxyls of serine and threonine residues of numerous cytoplasmic proteins, and is involved in many critical cellular processes. A microplate having a Ni ion captured through a chelation by nitrilotriacetic acid ligand (Ni-NTA) on its surface allows the monitoring of an OGT's enzymatic activity using an OGT substrate acceptor protein with a poly-histidine tag and its donor substrate, UDP-GlcNAz. Ni-NTA-coated plate is efficiently blocked by a commercially available immunobot blocking buffer. In this study, thorough examinations of Ni-NTA-coated microplate have revealed its properties and led to optimize the solid-based assay method of the OGT's enzymatic activity.

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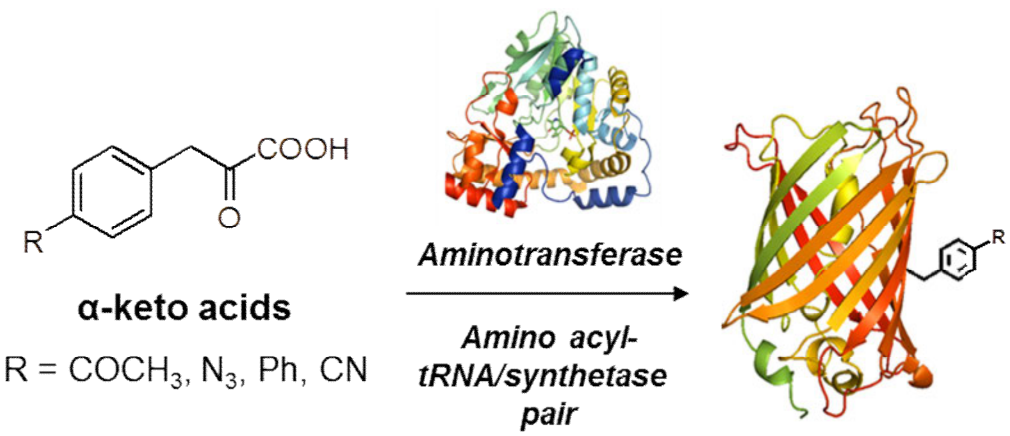
Genetic incorporation of unnatural amino acids biosynthesized from α-keto acids by an aminotransferase

고우석 이현수*

서강대학교 화학과

Four unnatural amino acids (UAAs) were synthesized from their corresponding α-keto acids by using glutamine:phenylpyruvate aminotransferase (GlnAT) from Thermus thermophilus HB8. The enzyme efficiently catalyzed the conversion of the unnatural substrates, with little decrease in its activity compared to that shown toward its natural substrates. The α-keto acids were converted into the corresponding amino acids in cells and then directly incorporated into a protein with high efficiency and fidelity. Because α-keto acids have no chiral center and are synthetically readily accessible, this method will further enhance the genetic incorporation technology and may present a new approach to the preparation of optically pure UAAs. Considering the substrate promiscuity of the GlnAT observed in the study, this method can be applied to the genetic incorporation of other UAAs derived from Tyr or Phe, which constitute approximately 50% of the successfully incorporated UAAs. In addition, this study provides an impetus for the development of an autonomous unnatural organism that can synthesize and incorporate UAAs.



Transamination and genetic incorporation

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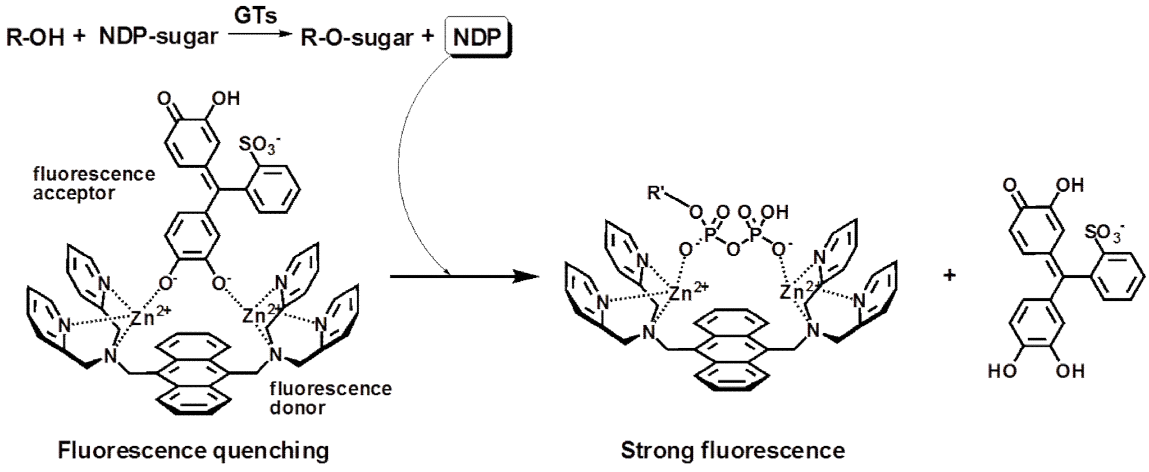
A fluorescence-based glycosyltransferase assay for high-throughput screening

고우석 이현수*

서강대학교 화학과

Glycosyltransferases catalyze the transfer of a monosaccharide unit from a nucleotide or lipid sugar donor to polysaccharides, lipids, and proteins in a stereospecific manner. Considerable effort has been invested in engineering glycosyltransferases to diversify sugar-containing drugs. An important requirement for glycosyltransferase engineering is the availability of a glycosyltransferase assay system for high-throughput screening of glycosyltransferase mutants. In this study, a general glycosyltransferase assay system was developed based on an ATP sensor. This system showed submicromolar sensitivity and compatibility with both purified enzymes and crude cell extracts. The assay system will be useful for glycosyltransferase engineering based on high-throughput screening, as well as for general glycosyltransferase assays and kinetics.



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Dopamine and Cu+/2+ can induce oligomerization of α-synuclein in the absence of oxygen: two types of related oligomerization mechanisms for α-synuclein

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한국과학기술원(KAIST) 화학과

It has been hypothesized and supported that α-synuclein oligomer can induce the toxicity in Parkinson's disease progression. Although many studies reported α-Syn oligomerization by dopamine (DA) and transition metal ions, there are few studies about joint influences of DA and Cu2+. In this study, DA and Cu2+ were co-treated for measuring of α-Syn oligomerization. In the presence of oxygen, DA induced α-Syn oligomerization in a dose-dependent manner. Cu2+ did not effect oligomerization in a dose-dependent manner in the presence of DA. By electrophoresis, Cu2+ ions are shown to change oligomers which were induced by DA into other types easily. This implies oligomerization reaction by DA is reversible in the presence of Cu2+. In the absence of oxygen, DA induced less oligomerization of α?synuclein whereas DA/Cu2+ induced aerobic?level amounts of oligomers. This suggests that DA/Cu2+ can induce oligomerization independent of oxygen. Radical species were detected through EPR analysis, from co?incubation of α?synuclein, DA and Cu2+. Redox reactions induced by DA/Cu2+ were observed in multimer regions of α-synuclein oligomers through NBT assay. From these results, we discussed DA and DA/Cu2+ induce different mechanisms on α-synuclein oligomerization: cross?linking versus radical?mediated covalent modification.

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The importance of insertion-in-flap (IF) domains in chaperone-linked amyloid fusion proteins

김수현 이경희*

세종대학교 화학과

α-Synuclein (αSyn) plays a key role in Parkinson’s disease and Iset amyloid polypeptide (IAPP) is associated with typeⅡ diabetes, triggering structural transitions from random coils or α-helices to β-sheet. In the previous study, FKBPIF (or F36VIF) chaperone proteins exhibit the faster amyloid fibril formation of αSyn, with the insertion-in-flap (IF) domain of SlyD hybridized. In order to further investigate mechanisms of the accelerated fibril formation of target proteins such as αSyn and IAPP, we have constructed recombinant fusion plasmids between chaperone domains (FKBP, FKBPIF, F36V and F36VIF) and amyloid proteins (αSyn or IAPP) with a linker of 23 amino acids (H6-chaperone?L23?amyloid). Fusion proteins were overexpressed by IPTG in E.coli and further purified by Ni2+- affinity chromatography and anion exchange chromatography, if necessary. We have measured thioflavin T (ThT) fluorescence to address the role of IF domains in regulating the rate of amyloid fibril formation, when fused.

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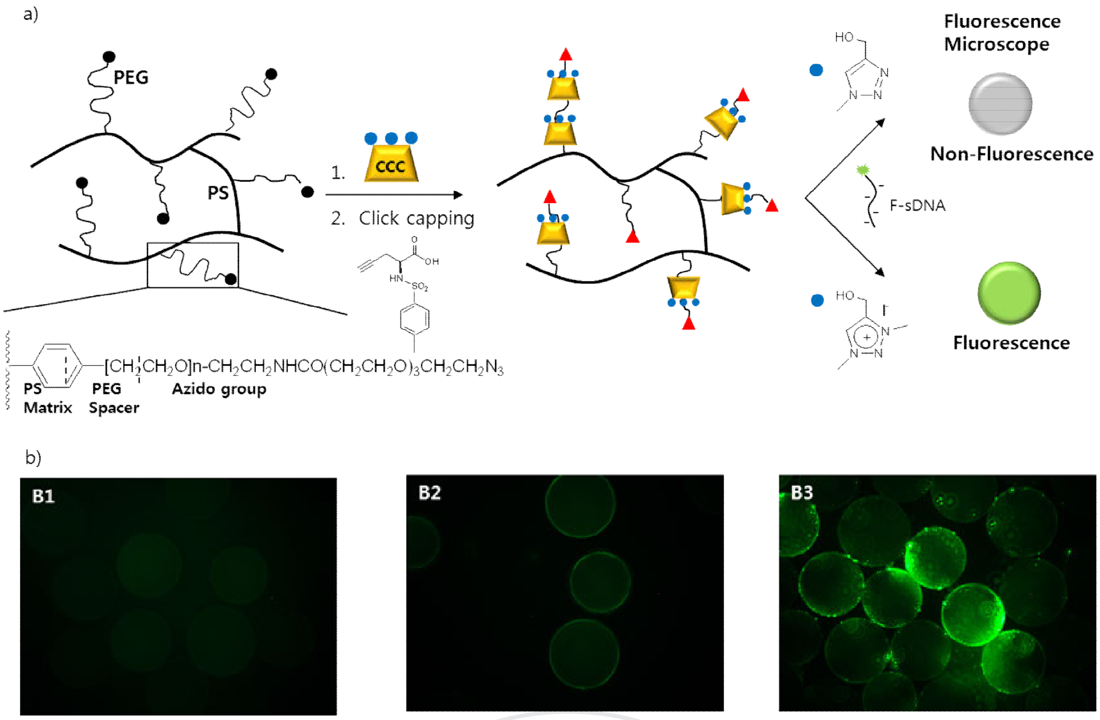
DNA complexation of triazolium-α-cyclodextrin

김태우* 송정은 강철훈* 위영진 Le Thi Hoa

경희대학교 동서의학대학원

Per-cationic cyclodextrins (CDs) were proposed to condense plasmid DNA. Stable complexes were reported between DNA and β-CDs with pyridylamino, alkylimidazole, methoxyethylamino or amino pendants. CDs bearing guanidinoalkylamino and aminoalkyl groups were reported as biomimetic structures of cell-penetrating peptides.However, DNA complexation of triazolium-α-cyclodextrins has not been investigated to our knowledge. A triazolium-α-cyclodextrin (T+-α-CD) was synthesized by methylation of 6-hydroxymethyltriazole-6-deoxy-α-cyclodextrin. T+-α-CD was characterized by ^{1}H, ^{13}C, HH-COSY, and CH HSQC. The cytotoxicity of T+-α-CD was measured by MTT assay. The DNA complexation of T+-?-CD was confirmed by turbidity test between T+-α-CD and double strand DNA. In addition fluorescein labeled single strand DNA was visualized on TentaGel resin, which was immobilized with T+-α-CD. The DNA complexation of triazolium-α-cyclodextrin can be explained by the multivalent electrostatic interaction between triazoliums and phosphates. Triazolium cyclodextrin will be an alternative, cationic cyclodextrin derivative useful for DNA complexation.


a)
PEG
PS
1.
CCC
2. Click capping
Fluorescence Microscope
Non-Fluorescence
F-sDNA
Fluorescence
HO
N
N–N
I⁻
[CH2CH2O]n-CH2CH2NHCO(CH2CH2O)3CH2CH2N3
PS Matrix
PEG Spacer
Azido group
OH
HN
SO2
b)
B1
B2
B3

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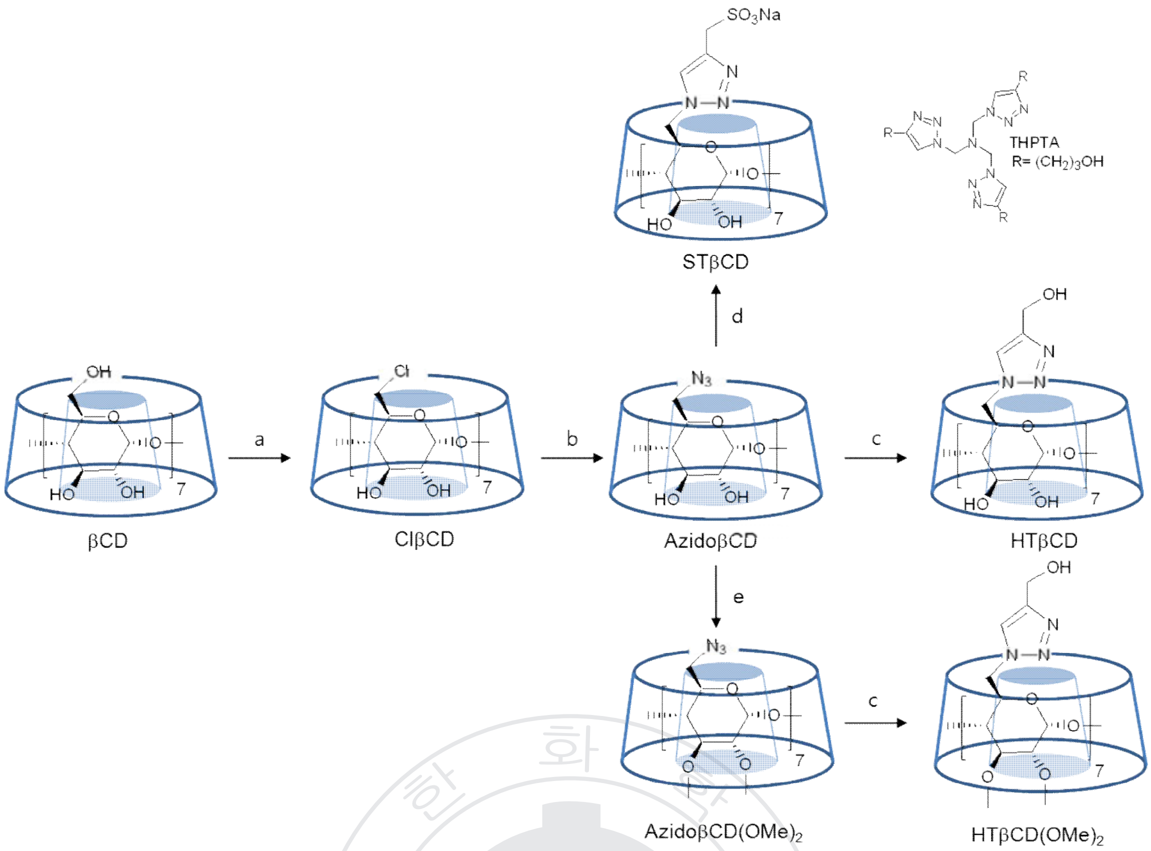
Synthesis, Cellular Toxicity, and Prednisolone Phase-Solubility Study of -[1,2,3]triazol-1-yl Cyclodextrins

김태우* 강철훈* **Le Thi Hoa** 윤영민 박영빈[1]

경희대학교 동서의학대학원 [1]경희대학교 동서의과학과

To explore the possibility of cyclodextrin click clusters (CCCs) as a new cyclodextrin-based excipient, we synthesized three different CCCs and investigated their water-solubility, cellular toxicity, and drug-solubilizing effect. HT-β-CD, HT-β-CD(OMe)2, and ST-β-CD were synthesized using copper(I)-catalyzed azide-alkyne cycloaddition from 6-azido-6-deoxy-β-CD. Water turbidity testing of the CCCs showed that the minimum water solubility of the CCCs is at least 20 times higher than that of β-CD. An MTT cell viability assay performed on HeLa cells demonstrated a low cellular toxicity of the CCCs compared with 2,6-dimethyl-β-cyclodextrin. HT-β-CD(OMe)2 and ST-β-CD did not demonstrate any cellular toxicity within the experimental concentration (~5 mM) like 2-hydroxypropyl-β-CD. A phase-solubility study of prednisolone with the CCCs suggested that CCCs showed increased solubility of prednisolone in the presence of increasing concentrations of the CCCs. The comparison between the conventional CD derivatives and CCCs on solubility, cellular toxicity, and binding property implies that CCCs are alternative cyclodextrin derivatives useful for overcoming the restrictions of conventional cyclodextrin chemistry.


SO3Na
STβCD
THPTA
R= (CH2)3OH
d
βCD
a
ClβCD
b
AzidoβCD
c
HTβCD
e
AzidoβCD(OMe)2
c
HTβCD(OMe)2
7

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Development of Image-based High-Throughput Screening System to Monitor Glucose Uptake in Living Cells

조아라 박승범*

서울대학교 화학부

We previously reported a novel fluorescent glucose analog, GB2, which is applicable to fluorescence-based real-time and quantitative monitoring of glucose uptake in living cells. Because glucose homeostasis plays an important role in human diseases, we aimed to develop a novel image-based screening system to monitor the perturbation of cellular glucose uptake in a high-throughput manner. The detailed mechanistic studies on the cellular translocation of GB2 led us to 2 important physiological characteristics: (1) the translocation of GB2 across the plasma membrane is mainly mediated by glucose transporters; (2) GB2 is not a substrate of HKs; therefore, GB2 is not retained in the cytoplasm after cellular uptake, and it is substantially released from the cell through GLUTs by a reversed concentration gradient. This is a crucial challenge for the development of a reliable image-based HTS assay with GB2 because the fluorescence signal might be misread owing to the inevitable difference of the detection time in large-scale screening. To address this issue, we used phloretin, a transient and selective GLUT inhibitor, for bioimaging to effectively suppress the efflux of GB2. With this breakthrough, we developed the first image-based HTS system to monitor the glucose uptake in living cells with robustness, reproducibility, and accuracy. Furthermore, we anticipate the application of our image-based phenotypic assay in HCS systems in conjunction with other orthogonal assays, including intracellular trafficking, signaling processes, and glucose utilization in living cells. Considering the high demands for the discovery of therapeutic agents in the treatment of diabetes, obesity, and cancer, our image-based HTS assay provides a powerful tool to identify novel hit compounds with a new mechanism of action.

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Solution Structure of *Enterococcus faecalis* Acyl Carrier Protein studied by NMR Spectroscopy

박영근 정기웅 김양미*

건국대학교 생명공학과

Fatty acid synthesis in bacteria is catalyzed by a set of individual enzymes collectively known as type II fatty acid synthase (FASII). Each enzyme interacts with acyl carrier protein (ACP), which shuttles the pathway intermediates between the proteins. *Enterococcus faecalis* is a commensal bacteria now acknowledged to be organisms capable of causing life-threatening infections in humans, especially in the nosocomial (hospital acquired) environment. Structure of acyl carrier protein from *E. faecalis* (Ef-ACP) has never been studied yet. To study the structural feature and thermal stability of Ef-ACP, we optimized cloning system and the expression condition of Ef-ACP. Using circular dichroism (CD) spectroscopy, Ef-ACP was characterized to have an alpha helical structure. Thermal stability was studied by measuring melting temperature and Ef-ACP showed melting temperature at 70°C, which is much higher than that of ACP from *Escherichia coli* (54°C). We performed multidimensional heteronuclear NMR experiments and completed the backbone resonance assignment. The mutagenesis study revealed that His17 and Phe45 contributed to structural stability of Ef-ACP conformations. Structures and dynamics of Ef-ACP and acyl-ACP will be further investigated by NMR spectroscopy to understand the specific recognition mechanisms between acyl-ACP and functionally different enzyme partners in fatty acid synthetic pathway.

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The Importance of loop Motions in Phosphatases of Regenerating Liver-3 (PRL-3)

정기웅 진봉환 김양미*

건국대학교 생명공학과

Phosphatases of regenerating liver (PRL) constitute a prenylated phosphatase with oncogenic activity. PRL-3 is overexpressed in liver metastasis of colorectal cancer cells, and it represents a new therapeutic target. With the aim of verifying the functional importance of the inherent structural flexibility of PRL-3, we investigated the structural and dynamic features of apo- and holo-PRL-3. Apo- and holo-PRL-3 have substantial differences in the general acid loop. Moreover, Cys104, Arg110, and Asp72, which participate in the enzymatic reaction, are close together in holo-PRL-3. Based on the spin relaxation, CPMG data and model-free analysis, we found that microsecond to millisecond time scale motions on the general acid loop and α5-α6 as well as P-loop are important in ligand recognition and the differences between loops flexibilities in apo- and holo-PRL-3 may control the protein-ligand interaction. Flexibility of PRL-3 shown in this study may be essential for its ability to dephosphorylate the enzyme partners.

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Function of three phenylalanines and Val^{10} in piscidin-1 on its mechanisms of antibacterial activities and cytotoxicities

이은정 신아름 김양미*

건국대학교 생명공학과

Piscidin-1 (Pis-1) is an antibacterial peptide derived from mast cells of hybrid striped bass that comprises 22 amino acids with phenylalanine-rich amino-terminal. To verify the key residues for the antibacterial activity and those for the cytotoxicity of piscidin, we investigate the role of each Phe residue as well as the Val^{10} which is located at the hydrophilic phase. Tryptophan fluorescence blue shift was monitored for the peptides with Trp substitution of Phe^{1}, Phe^{2}, and Phe^{6}, respectively. Each Phe was substituted with Ala or Lys to investigate their functional roles. As results, and Phe^{2} plays key roles in cytotoxicity of Pis-1 while Phe^{2} and Phe^{6} plays key roles in antibacterial activities of Pis-1. We also designed piscidin analogue, Pis-V10K with Lys substitution of Val^{10} which results in an elevated amphipathic α-helical structure showed similar antibacterial activity when compared with Pis-1; however, it showed much lower cytotoxicity than Pis-1. NMR spectroscopy revealed that Pis-V10K in a 300 mM SDS micelle had a linear amphipathic alpha-helical structure from Phe^{2} to Thr^{21}. In this study, we have demonstrated that piscidin analogs which substituted with Lys in Pis-F1K/V10K and Pis-F2K/V10K are potent peptide antibiotics with both anti-inflammatory and antimicrobial activities and we provide mechanism of action of piscidin analogs.

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Relationship between Structure and function of hybrid antimicrobial peptide, Papiliocin(Pap)-Magainin(MA)-P2 and its analogs

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Papiliocin is consisted of 37-amino acids antimicrobial peptide which is purified from the swallowtail butterfly, Papilio xuthus. Magainin 2 is consisted of 23-amino acids antimicrobial peptide which is isolated from African clawed frog. PapMA is a 20-residue hybrid peptide incorporating residues 1-8 of papiliocin and residues 1-12 of magainin 2. PapMA have potent antimicrobial activity without toxicity against mammalian cells. PapMA-P2, in which the Gly-Ile-Gly sequence of PapMA is substituted with Pro, was designed. According to the results of cytoxicity against bacteria and mammalian cells, and phospholipid membrane permeability, PapMA-P2 with high antimicrobial acitivities targets the bacterial cell membrane. To discover peptide antibiotics having lower toxicity and higher selectivity, we substituted ala, lys and leu peptoids for Pro. Peptoid analogues also showed that high antimicrobial activities and low toxicities against mammalian cells. CD spectra and NMR spectroscopy suggested that PapMA-P2 and its analogues have α-helical conformations in membrane-mimicking environment. PapMA-P2-lys peptoid exists in dynamic equilibrium of cis and trans conformers with a ratio of 1:3. Structure-activity relationships of these peptides will give insights to understand its mechanism of actions and help to develop more potent peptide antibiotics as useful therapeutic agents.

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발표종류: 포스터, 발표일시: 수 16:00~19:00

Structural and Functional properties of the Thermophilic Cold Shock Protein from *Thermus Aquaticus*

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건국대학교 생명공학과

Csps are proteins expressed when growth temperature drops below physiological temperature. They bind to single-stranded nucleic acids and play a central role in the regulation of gene expression under cold shock conditions as RNA chaperones. Here, in order to understand the structural feature of Csp from a thermophilic bacterium, *Thermus aquaticus* (Ta-Csp), we investigate the thermal stability of Ta-Csp by circular dichroism (CD) experiment. Ta-Csp is more thermostable with higher melting temperature (76˚C) compared with mesophile, *Escherichia coli* Csp (60˚C) and psychrophile, *Listeria monocytogenes* Csp (40˚C). The structural study of Ta-Csp showed that the longer β strands and more hydrophobic core packing as well as favorable electrostatic interactions may be key factors in determining the high thermostability of Ta-Csp. Upon binding heptathymidine (dT_7), heteronuclear NOE values and order parameters of residues in surface loop regions dT_7 binding sites increased dramatically. Moreover, Carr-Purcell-Meiboom-Gill experiments showed that slow motions observed for the dT_7 binding residues K7, W8, Y15 and F30 disappeared in Ta-CspA-dT_7.

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Development of inhibitory peptide as an antifungal agent towards *Phytophthora capsici* microtuble

윤문영

한양대학교 화학과

Phytophthora blight of pepper caused by an oomycete pathogen *Phytophthora capsici(P. capsici)* and is responsible for major losses in pepper production and the pathogen can survive in soil in the absence of the host plant for many years. Microtubules have several key roles that are important in cell proliferation, trafficking, signaling and migration in eukaryotic cells. Due to these reasons microtubule is an attractive target of many antifungal agents. In this study, we screened alpha and beta tubulin binding peptides from *Phytophthora capsici* by phage display method. After five rounds of biopanning, we identified peptides showed picomolar range of high binding affinity from a random peptide library toward *P. capsici* alpha and beta tubulin. The specificity of peptides was found 78% higher compared to bacterial FtsZ from *Xanthomonas axonopodis*; which has similar role to that of eukaryotic tubulin. Among them, a couple of peptides showed high inhibition against microtubule formation with IC50 in the range of 890 nM ? 1.3 μM concentration which is much lower than well-known chemical inhibitor Benomyl (IC50 = 500 μM). Based on these results, it is anticipated that these peptides could further be used promising candidate as novel antifungal agent against *Phytophthora* blight disease.

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Identification of a novel potent antibacterial agent against*Mycobacterium tuberculosis*Acetohydroxyacid Synthase

문지영 하나름 윤문영*

한양대학교 화학과

Mycobacterium tuberculosis acetohydroxyacid synthase (MTB-AHAS) is a potential and promising candidate in the development of novel anti-tuberculosis drugs. AHAS from MTB is one of the biosynthetic enzymes, which catalyzes the first common step in the biosynthesis of the essential branched chain amino acids (BCAA's: valine, leucine, and isoleucine). To identify new inhibitory scaffolds, we used a high-throughput screening and tested a chemical library composed of 6500 compounds (from KRICT). The screen identified 15 compounds, each representing a structural class, as MTB-AHAS inhibitors with an IC50 in the low micro molar range (0.4?7μM). The inhibitors demonstrated non-competitive, un-competitive or mixed competitive inhibition. Further, molecular docking of potent chemicals in MTB-AHAS yielded ?8.5 ~ ?11 kcal/mol (ΔG) binding energies, respectively. The binding modes were consistent with inhibition mechanisms, as both chemicals oriented outside the active site. This potent inhibitor might provide an impetus for the development of a strong anti-tuberculosis agent targeting *M.tuberculosis* AHAS.

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Direct Oxidative Esterification of Aldehydes Using UHP and Aluminum chloride hexahydrate in Alcohols

이신애 이종찬*

중앙대학교 화학과

Esters are one of the most valuable organic functionality and have immense importance in organic and pharmaceutical chemistry.Numerous synthetic methods are known for the transformation of aldehydes into the corresponding esters. However, these methods required use of toxic reagents, harsh oxidants, expensive reagents, difficult to prepare transition metal catalysts.Herein, we disclose the oxidation of aldehydes to the corresponding esters using UHP and aluminum chloride hexahydrate in excellent yields.The oxidation of various aldehydes into corresponding esters was carried out in alcohols as solvent in the presence of an aluminum chloride hexahydrate and urea hydrogen peroxide(UHP) as oxidant at 60℃ in 5~12h.Both electron-donating and electron-withdrawing functional group in aromatic rings give equal well high yields.In conclusion, our work is a highly efficient, cost-effective, eco-friendly, mild, simple protocol for the one-pot oxidative esterification of aldehydes using UHP and aluminum chloride hexahydrate in alcohols.

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Synthesis of cyanocombretastatin analogues for anticancer agents

유정원 민동국 정만길*

연세대학교 화학과

In many classes of stilbinoid natural products, combretastatins are exceptionally potent inhibitors of cell division. They have been found to be a prominent inhibitor of tubulin polymerization and a cytotoxic agent against a wide variety of human cancer cell lines, including multi-drug resistant cell lines. Also, as combretastatins can dock into the colchicine binding site of tubulin, they have a potent antimitotic property. According to many researches, combretastatins which have a nitrile function on the olefinic bond, represent the increased cytotoxicity, water solubility and antiproliferative activity. In this study, we have synthesized novel cyanocombretastatin derivatives for a notable anticancer agent. In addition, we have introduced nitrovinyl moiety which possesses a proapoptotic effect into cyanocombretastatin derivatives for anticancer agents.

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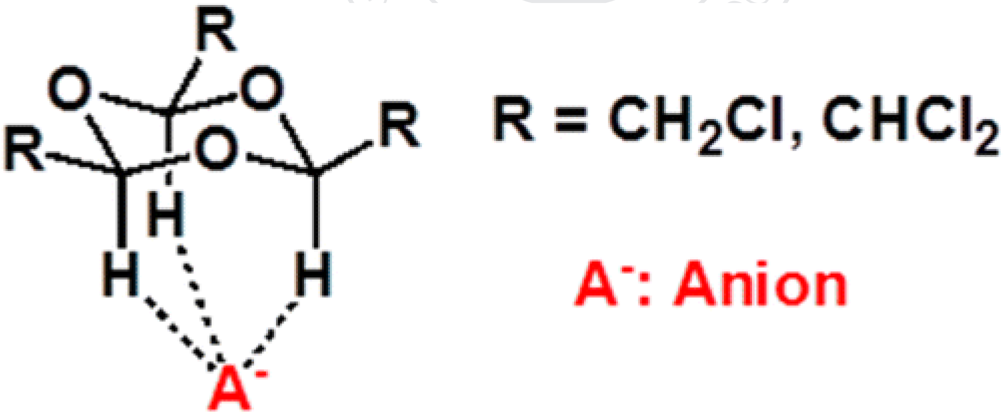
Novel Anion Receptors with 2n-Crown-n Topology

조승주

조선대학교 의학과

A series of novel coronands having a 2n-crown- n topology based on trioxane (6-crown-3) derivatives are designed and characterized. These neutral hosts can sense anions through pure aliphatic C?H hydrogen bonding (HB) in condensed phases due to the unusual topology of 2n-crown-n. C?H bonds are strongly polarized by two adjacent oxygen atoms in this scaffold. These hosts provide a rare opportunity to modulate anion binding strength by changing the electronic nature of aliphatic C?H bonds and offer ease of synthesis.Reference: Shi, G. et al. Org. Lett. 2014, 16(2), 334-337.



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Synthesis of Daumone-Chalcone hybrid

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연세대학교 화학과 [1]연세대학교 화학과

Daumone is a glycolipid pheromone of Caenorhabaditis elegans inducing dauer state, and have been reported that it has anticancer activity comparable to doxorubicin. Chalcone derivatives, precursors for different classes of various flavonoids, have also been reported that it has biological activities such as brain dysfunction, cancer, infection and cardiovascular risk. In this study, we have synthesized new daumone-chalcone hybrid compounds for anticancer activities because hybrid drugs is expected to impact multiple targets simultaneously, so they are less prone to drug resistance and the standard of care in cancer treatment.

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A Study on the Selectivity of Arylzinc Reagents in Cross-coupling Reactions with Chemically Equivalent and Pseudo-equivalent Dibromopyridines

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단국대학교 화학과

Heterocyclic compounds bearing a pyridine moiety have shown a broad range of biological activities as a result of diverse substitutents containing numerous different types of functionalities. Consequently, new practical synthetic approaches for constructing pyridine complex molecules are of high value. To this end, transition-metal-catalyzed crosscoupling reactions of various organometallics with halopyridines have been frequently utilized as one of the efficient protocols. In spite of the high value of using halopyridines, recent researches have been intensively focused on the site-selective cross-coupling reactions with organometallic reagents because the most of pyridine derivatives found in natural compounds and material chemistry have at least two different types of substitutents on a pyridine ring.

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Tuning lateral packing densities of pOEGMA on gold surfaces and its impact on the amount of immobilized streptavidin

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Biofouling, the accumulation of biological matters on a surface causing the deterioration of the device, is a problematic issue in a wide range of fields, such as biomedical devices/implants, biosensors, drug delivery carriers, and food industry. Recently, specific immobilization of biomolecules on non-biofouling polymeric films has received much attention, because it can serve as a platform for achieving highly sensitive biochips and biomedical devices. Previously reported results not only indicated that the amount of immobilized protein can be controlled by selection of reactive sites, but also encourage us to understand binding behaviors. Thus, we investigated binding behaviors of streptavidin with the different lateral packing densities of biotin-functionalized, non-biofouling pOEGMA brushes. pOEGMA was synthesized by surface-initiated polymerization from the mixed SAMs with different mole fractions of initiators on gold surfaces.

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Air Oxidation of beta-Ketoesters by Mn(III)/Co(II) Catalyst and Consecutive Conversion to Heterocycles

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Mn(OAc)3 has been known to act as a radical initiator of carbonyl compounds to react with carbon-carbon double bonds to complete cyclization. The mechanism of the novel oxidative deacetylation method of acetoacetates triggered by Mn(OAc)3 was reported. However, the mapping details of the whole sequence needed to be further investigation. After the detailed screen, the reaction can be successfully carried out under 5mol% Mn(OAc)3 and 2mol% CoCl2 in ethanol at 60 ºC in good yield. Furthermore, with the amine resources inside the reaction system, hetero-5-member-ring can be obtained successfully. This method can be applied to a novel one-pot synthesis of pyrrole and indole derivatives.

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A study on the synthesis of various 2,7-substituted-oct-4-enedials as a key subunit for Unnatural Carotenoids

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The carotenoids are important class of organic molecules with delocalized π-electrons, which show electric conductance. We synthesized the titled dials by coupling 1,4-dibromo-2-butene and 2-substituted acetate, followed by LiAlH4 reduction and swern oxidation. The unnatural carotenoids can be assembled our sulfone-mediate coupling and double elimination strategy utilizing by allylic sulfone and the above-mentioned dials. The conjugated polyene chains of the unnatural carotenoids containing aromatic substituents would offer an extra stability and excellent electronic characteristics compared with those of the natural carotenoids.

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Efficient Synthesis and Structural-Mechanistic Investigation of N-Aryl Fructosamines: Scope and Limitations

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Synthesis of N-Aryl Fructosamines using Amadori reaction from D-glucose with aromatic amines has been accomplished with two-step procedure. Study towards the structure of the synthesized products and mechanistic investigation of the reaction also been performed. The process finds the efficient way of synthesizing fructosamines in enantiomerically pure form useful as chiral building blocks.

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A study of Allylic sulfone synthesis for the unnatural carotenoids

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Carotenoids have a structural characterics of conjugated polyene chains, which would be utilized as excellent materials for conductive organic molecules, organo-electric circuit, etc. We found that stability and electronic characteristics of the unnatural carotenoids containing aromatic substituents were superior to those of the natural carotenoids. Carotenoids can be obtained by coupling with allylic sulfones and dialdehyde. Chloro sulfone unit is the key compound for the allylic sulfone, which contain aromatic substituents, which can be prepared from the acetophenone derivatives. Allylic sulfone was prepared by Indium mediated addition of chloro sulfone unit to aldehyde followed by Oxonia-cope rearrangement.

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발표종류: 포스터, 발표일시: 수 16:00~19:00

Research on the synthesis of Unnatural carotenoids

임보람 구상호[1,*]

명지대학교 에너지융합공학과 [1]명지대학교 화학과

Unnatural carotenoids containing various phenyl substituents show excellent characteristics in terms of stability as well as electronic conductance. We have developed a series of efficient synthetic methods of natural carotenoids, which can be further extended to the synthesis of the unnatural stabilized carotenoids as a molecular wire. Our synthetic strategy is based on the sulfone-mediated coupling with dialdehyde and double elimination reaction. Under the sequence of Indium mediated addition of haloallylic sulfone and Oxonia-cope rearrangement reaction, allyic sulfone unit containing aromatic substituents can be readily prepared from acetophenone derivatives. The unnatural carotenoids can be synthesized by the coupling/double elimination reaction between allylic sulfone and dialdehyde unit. Therefore, we were able to measure electrical conductivity for the unnatural carotenoid wires.

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N-glycosylaion vs Amadori reaction of glucose

권순정 구상호[1,*]

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Biomass such as glucose and fructose can be converted to commodity chemicals (e.g. 2,5-FDCA, 2,5-DFF, 5-HMF, etc.) which can be used as energy material and drug intermediates. It is a potential and promising object to efficiently synthesize the glucose containing nitrogen compounds. Amadori rearrangement and N-glycosylation reactions are efficient tools for the synthesis of the above compounds which can be proceeded from the same substrates. The study on the control of the reaction conditions leading either to N-glycosylation or to Amadori has been carried out. The concentration of the acid on the product yield is examined in order to determine the optimum conditions for Amadori rearrangement. The control of temperature is more important than the amount of acid in the optimization of the Amadori product.

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Study on the preparation and self-assembly behavior of phosphatidylcholines of 1,2- vs 1,3-diglycerides

최정애 구상호[1,*]

명지대학교 에너지융합공학과 [1]명지대학교 화학과

Phosphatihylcholine is one of the major components of cell membranes.Phophatidylcholine is composed of a hydrophilic head group and two hydrophobic fatty acids parts. We replaced one of the fatty acid part with α-tocopherol.We were able to synthesize regioisomeric diglycerides by the regioselective epoxide ring opening with acid nucleophiles, which were efficiently utilized for the formation of diversely substituted phosphatidylcholine derivatives.Self-assembly patterns of phosphatidylchoine compounds in aqueous solution were studied by optical microscopy.we found interesting results depending on the regioisomeric diglycerides.

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NHC/Chinchonine Dual Catalytic System for the Asymmetric Synthesis of 3-Substituted Phthalides

송형섭 유현지 윤소원*

한양대학교 화학과

Asymmetric domino multicatalysis has been emerging as a highly efficient and powerful method for the synthesis of structurally complex molecules from relatively simple starting materials. Recently, we developed a highly efficient NHC-catalyzed domino oxidation/oxa-Michael addition reaction of *o*-alkenylbenzaldehydes that enabled the easy preparation of a diverse array of 3-substituted phthalides. Chiral 3-substituted phthalides are important classes of naturally occurring lactones that have been found to exhibit a wide range of biological indications and to be versatile building blocks for the synthesis of bioactive compounds. In light of our recent success in NHC-catalyzed domino oxidation/oxa-Michael addition reaction of *o*-alkenylbenzaldehydes, we investigated a dual catalytic system consisting of an achiral NHC and chiral bifunctional cinchonine for the synthesis of chiral 3-subtituted phthalides.

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Ag(I)-Mediated Indole Synthesis

고태윤 장수산 윤소원*

한양대학교 화학과

Indole has been used in various areas for decades, especially in pharmaceutical industry because of their biological activity. Recently we have investigated the Ag(I)-mediated intramolecular cyclization reaction for the synthesis of indole derivatives. We optimized the reaction conditions through screening studies of Ag salts, solvents, and reaction temperature.

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발표종류: 포스터, 발표일시: 수 16:00~19:00

Pd-Catalyzed Oxidative Intramolecular C-H Amination

정은주 윤소원*

한양대학교 화학과

Transition-metal-catalyzed intramolecular oxidative aminations of the C-H bond have emerged as important methods for C-N bond formations because of economical advantages over the present procedures by employing prefunctionalized substrates. In particular, Pd-catalyzed C-H aminations have emerged as powerful tools for the synthesis of a number of unique heterocycles. In this context, we have investigated a Pd-catalyzed C-H amination of (*Z*)-*N*-protected dehydroamino acids. We will demonstrate our findings regarding the optimization study and substrate scope.

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The Synthesis and properties of Rhodamine derivatives Phenothiazine sensors

손문수 장승현*

대구대학교 화학과

In this research, we have synthesized the compound 1,2 and compound 3 from phenothiazine containing rhodamine 6G derivatives. The synthetic routes for the phenothiazine derivatives and rhodamine 6G derivatives are outlined in scheme 1. The imine reaction of two derivatives were synthesized. The structures of all reaction products were confirmed by ^{1}H-NMR, FAB-Mass, GC-Mass. New compounds were found selectivity for metal cation by fluorescence titration using various metal cation.

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발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis and properties of perlyene containing rhodamine6G motiety

장은수 장승현[1,*]

성균관대학교 화학과 [1] 대구대학교 화학과

Perlyene containing rhodamine 6G was perpared by two step. Step one, rhodamine 6G containing ethylenediamine was synthesized by ethylenediamine and rhodamine 6G in ethanol solvent. Step two, rhodamine 6G ethylenediamine containing perlyene was synthesized by perlyene and rhodamine 6G ethylenediamine in DMSO solvent. The structure of all reaction product were confirmed by ^{1}H-NMR, GC-Mass.

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발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis and fluorescence properties of Rhodamine 6G derivatives

최재영 장승현*

대구대학교 화학과

We synthesized new kinds of bis type of rhodamine fluorescent sensors.Compound 1 was synthesized from rhodamine 6G and 1,3-diaminopropane derivative and 1,4,5,8-naphthalene tertracarboxilic dianhydride. Compound 2 was synthesized from rhodamine 6G and 1,4-diaminobutane derivative and 1,4,5,8-naphthalene tertracarboxilic dianhydride. Synthesis, fluorescence properties will be discussed. These synthesized compound were confirmed by ^{1}H-NMR, FAB-Mass and selectivity, complexation of metal measured in the fluorescence spectrum.

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Non-covalent Interactions Existed in Octameric β-Peptide Foldectures

공진택 이희승*

한국과학기술원(KAIST) 화학과

Recently we have published unprecedented shapes of β-peptide self-assembled structures which were named foldecture (i.e. self-assembled foldamer)[1]. Study on the formation mechanism of foldecture is expected to give an intuition of formation process of various 3D materials in nature, such as protein folding. As the first step of the study, understanding of its molecular packing structure is essential. For this purpose, SDPD technique has been applied to foldectures.

Herein we present the result of structural analysis of a finite plate-shaped foldecture that was obtained by controlled self-assembly of $ACPC_8$ and $ACPC_6Leu_2$ foldamers in aqueous solution, respectively. The molecular packing structures showed orthorhombic system, which clearly indicated three-different ways of molecular interaction in each a, b and c axis. The similar packing structures of both β-peptide foldectures indicate resemblance of formation process of the foldectures, which resulted in finite plate-shape.

References

1.(a) S. Kwon.; H.S. Shin.; J. Gong.; J.-H. Eom.; A. Jeon.; S.H. Yoo.; I.S. Chung.; S.J. Cho.; H.-S. Lee. J. Am. Chem. Soc. 2011, 133, 17618. (b) J. Kim.; S. Kwon.; S. H. Kim.; C.-K. Lee.; J.-H. Lee.; S. J. Cho.; H.-S. Lee.; H. Ihee. J. Am. Chem. Soc. 2012, 134, 20573. (c) S. Kwon.; A. Jeon.; S. H. Yoo.; I. S. Chung.; H.-S. Lee. Angew. Chem. Int. Ed. 2010, 49, 8232.2.W. A. Dollase. J. Appl. Cryst. 1986, 19, 267.

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Iridium Catalyzed Single-Step N-substituted Lactam Synthesis from Lactones and Amines

김기철 홍순혁*

서울대학교 화학과

A novel catalytic lactam synthesis under a mild condition was developed with [Cp*Ir] complex. Within the method, amide bond and C-N bond formation occur in one-step reaction. Three subsequent transformations - aminolysis of lactone, N-alkylation of hydroxyl amide with amine, and transamidation of amino amide- furnish N-substituted lactam.

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Revealing copper-overloaded endoplasmic reticulum by using novel fluorescent organelle-selective Cu^{2+} ion probes

이윤학 윤병권 선우경 강철훈[1,*] 김종승[*]

고려대학교 화학과 [1]경희대학교 동서의학대학원

Copper ions play essential roles in various biological systems and its homeostasis is tightly controlled in the mammalian cells. However, imbalances in copper homeostasis are responsible for defects in copper export systems and central nervous system in Wilson's disease as a genetic disorder by mutated ATP7B gene. Copper toxicity may contribute to the generation of reactive oxygen species (ROS), which can lead to cellular damage, oxidative stress and DNA damage. Its cytotoxic effects may involve malfunction of various organelles although the excess of copper ions is mainly accumulated in lysosome in the hepatocytes. However, its effect on subcellular organelle functions or copper uptake pathways is poorly understood. Therefore, we present the synthesis and development of organelle-selective fluorescent Cu^{2+} sensors, 1 and 2, bearing naphthalimide and dipicolylamine (DPA) units. Confocal microscopic images indicated that probes 1 and 2 are mainly localized in ER and lysosome, respectively. Upon addition of the excess copper ions to the living cells, probe 1 showed strongly quenched fluorescence intensity. Furthermore, inhibition of copper export system by sodium metavanadate ($NaVO_3$), aggravates fluorescence quenching of probe 1, suggesting that the ER is the primary site for copper reservoir in the overloading condition. Therefore, organelle selective probe 1 could be a valuable tool to understand the detailed role of copper ions. In addition this approach could be applied to diagnose pathogenesis related to the copper ion level changes.

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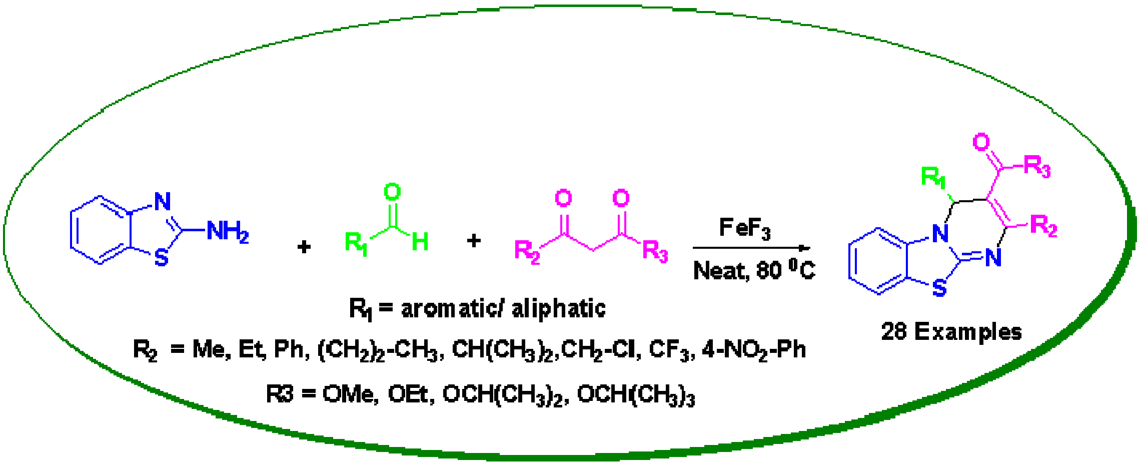
A facile green synthesis of differentially substituted triheterocyclic benzothiazole functionalities using iron fluoride under solvent free conditions

Atar Amol Balu 현동균 정연태*

부경대학교 이미지시스템공학과

A series of diverse polyfunctionalized triheterocyclic benzothiazoles were easily prepared in excellent yields via Biginelli reaction of 2-aminobenzothiazole with substituted benzaldehydes and α-methylene ketones using FeF3 as an expeditious catalyst under solvent free conditions. The protocol provides a practical and straightforward approach toward highly functionalized triheterocyclic benzothiazole derivatives in excellent yields. The reaction was conveniently promoted by FeF3 and the catalyst could be recovered easily after the reaction and reused without any loss of its catalytic activity. The advantageous features of this methodology are high atom-economy, operational simplicity, shorter reaction time, convergence, and facile automation.



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Novel blue organic-light emitting materials based on 9-(9,9-dimethyl-9H-fluoren-2-yl)-anthracene with triphenylsilane unit

송지영 박수나 이슬비 김찬우 윤승수*

성균관대학교 화학과

Four deep-blue-emitting materials based on anthracene and fluorene hybrids with triphenylsilane unit was synthesized and characterized to serve as blue emitting materials via Suzuki-coupling reaction for organic light-emitting diodes (OLEDs) application. Triphenylsilane unit could interrupt intermolecular interaction and reduce self-aggregation through steric hindrance of the non-planar structure. Also, we investigated conjugation-length effect through various connection form of anthracene and fluorene hybrids. To explore their electroluminescent properties, devices with the structure of ITO(180nm)/ NPB(50nm)/ blue materials (30nm)/ Bphen (30nm)/ Liq(2nm)/ Al (100nm) were fabricated. All devices showed deep-blue emission which suggested that triphenylsilane moiety effectively prevented intermolecular interaction and thus reduced concentration quenching in emitting layer. In particular, the device using S-3 exhibited high efficiencies (2.53 cd/A, 1.94 lm/W, 1.72% at 20mA/cm^2). These results demonstrated that triphenylsilane-substituted anthracene and fluorene hybrids might become candidates as emitting materials applied as OLED application.

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1,8-Naphthalimide based Bimodal Contrast Agent for Cellular Cu^{2+} Imaging

장주희 신원섭 박소연 김종승*

고려대학교 화학과

Magnetic resonance imaging (MRI) is an important imaging in diagnostic medicine. It provides high-quality three-dimensional images of tissue and anatomical resolution without use of injurious ionizing radiation. Gadolinium-based chelates are the most commonly used MRI contrast agents because the chelated Gd^{3+} metal ion enhanced MR signal by decreasing the longitudinal relaxation time (T1). As a result, T1-weighted MR image is brighter. We developed metal ions induced MR/Fluorescence signal enhanced bimodal imaging agent by taking of 1,8-naphthalimide framework with appended DTTA as Gd^{3+} chelating site. MR signal was enhanced in presence of biologically relevant target metal ions and fluorescence signal also altered. This dual modulated contrast agent can be used as cationic sensor which is a new biocompatible detector for biologically relevant metal ions to detect them in a noninvasive manner.

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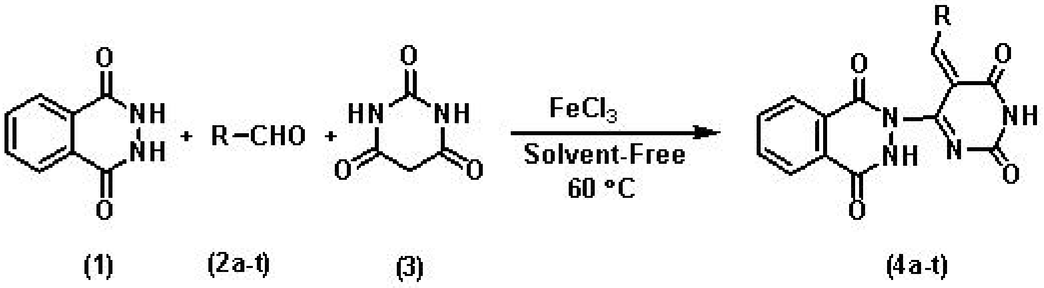
Synthesis of pyrimidin-4-yl)-2,3-dihydrophthalazine-1,4-diones catalyzed by FeCl3

<u>Mudumala Veeranarayana Reddy</u> 정연태*

부경대학교 이미지시스템공학과

Three-component coupling (3CC) of phthalhydrazide, aldehydes and barbituric acid has been accomplished in the presence of 15 mol % FeCl3 under solvent-free conditions to afford the corresponding synthesis of pyrimidin-4-yl)-2,3-dihydrophthalazine-1,4-diones in good yields. This method provides high yields, shorter reaction time and mild reaction conditions.



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FeCl3.SiO2: A new, highly efficient and recyclable catalyst for the synthesis spirooxindoles in aqueous media

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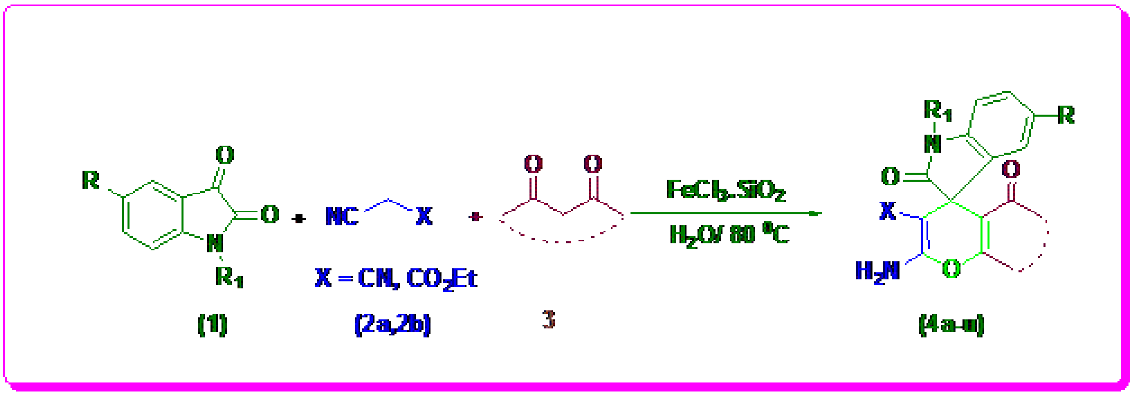
부경대학교 이미지시스템공학과

Silica supported ferric chloride one-pot three component synthesis of biologically active spirooxindoles was carried out by the reaction of isatin, malononitrile /ethyl cyanoacetate and cyclic 1,3-dicarbonyl compounds in aqueous medium. The salient features of this method are simple and convenient procedure, less reaction time, good reactive catalyst and excellent yield. The catalyst is recycled and reused with unchanged yield.



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Preparation of Benzoxaphosphole 1-Oxides through Rhodium-Catalyzed Oxidative Cyclization of Arylphosphonic Acid with Alkenes

류태규 김재은 박영철 김상혁 신서현 이필호*

강원대학교 화학과

C-H bond functionalizations catalyzed by transition metals have been demonstrated to be a very streamlined method for the formation of C-C and C-heteroatom bonds. In particular, *ortho* C-H bond functionalizations can be accomplished by the employment of a variety of directing groups with the aid of coordination of transition metals. In a number of directing groups for C-H bond functioalizations, nitrogen-containing compounds, carboxyl and hydroxyl ones have been broadly investigated. We report for the first time rhodium-catalyzed tandem oxidative alkenylation and intramolecular *oxa*-Michael reaction using arylphosphonic acid monoethyl esters and alkenes under aerobic conditions, which produced benzoxaphosphole 1-oxides in good to excellent yields.

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Synthesis of Phosphaisocoumarins through Rhodium-Catalyzed Oxidative Coupling of Arylphosphonic Acid mono-Esters with Alkynes

박영철 류태규 박상준 김철의 이필호*

강원대학교 화학과

A rhodium-catalyzed cyclization using alkynes and arylphosphonic acid monoesters for the synthesis of phosphaisocoumarins is reported. A range of substrates were selectively cyclized in high yield with functional group tolerance. Additionally, unsymmetrical alkynes are applied in high efficiency and regioselectivity. Mechanistic studies indicate that C?H bond metalation is irreversible and a rate-determining key step.

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Oxidative Cyclization of Phosphinic Acids and Phosphonic mono-Esters with Alkynes by Rhodium-Catalyzed C-H Activation

박영철 박상준 유은정 손정유 이필호*

강원대학교 화학과

The rhodium-catalyzed cyclization of phosphinic acids and phosphonic mono-esters with alkynes has been developed. A range of both diarylphosphinic acid and arylphosphonic mono-ester were selectively cyclized in high yield with excellent functional group tolerance. Additionally, we found that alkenylphosphonic mono-esters proceed smoothly to afford corresponding phosphorus 2-pyrones through oxidative annulations with alkynes. Mechanistic studies indicate that C-H bond metalation is irreversible and a rate-determining key step.

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C-H Activation/Cyclization for the Synthesis of Phosphaisocoumarins Catalyzed by Ruthenium

박영철 신서현 민지애 이필호*

강원대학교 화학과

An efficient and cost-effective ruthenium-catalyzed oxidative cyclization of phosphonic acid mono-esters or phosphinic acids with alkynes is developed for the synthesis of a wide range of phosphaisocoumarins in good to excellent yields under aerobic conditions. A multitude of arylphosphonic acid mono-esters and arylphosphinic acids having electron-donating and -withdrawing groups were oxidatively cyclized. Various diarylacetylenes, dialkylacetylenes, and alkyl arylacetylenes underwent effectively the ruthenium-catalyzed oxidative cyclization. Substrate possessing benzoic acid as well as phenylphosphonic mono-ester moiety was smoothly cyclized with hex-3-yne to afford compound having both isocoumarin and phosphaisocoumarin moiety. Alkenylphosphonic mono-ester afforded phosphorus 2-pyrone through oxidative cyclization with alkyne. Competition experiments between diaryl and dialkyl-alkynes and between diarylacetylenes having *p*-methoxy and *p*-chloro group gave the results that the present oxidative cyclizations were not affected by electronic effect of alkynes. Mechanistic studies revealed the C-H bond metalation to be rate-limiting step.

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발표종류: 포스터, 발표일시: 수 16:00~19:00

Oxidative Alkenylation of Arylphosphine Oxides by Rhodium-Catalyzed C-H Bond Activation

모준태 박상준 류태규 김상혁 이필호*

강원대학교 화학과

C-H activation reaction catalyzed by transition metals has emerged as an atom- and step- economical synthetic method and its synthetic applications have been proved in the preparation of natural products, pharmaceuticals, and organic materials. Recently, we have focused on phosphoryl-related compounds as the directing group for C-H activation. However, the employment of arylphosphine oxide as directing group have been rarely reported. Therefore, development of new C-H activation using phosphorus-related directing group is challenging. We report an efficient rhodium-catalyzed oxidative *ortho*-alkenylation of arylphosphine oxides with activated as well as non-activated alkenes with functional group tolerance. Current efforts are directed toward the development of efficient reactions using phosphorus-related functional group and their application.

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Synthesis of Phosphacoumarins by Gold-Catalyzed Hydroarylation

김철의 류태규 김상혁 이창희 이구연[1] 이필호[*]

강원대학교 화학과 [1]강원대학교 생명건강공학과

Organophosphorus compounds have been received continuous interests due to their frequency in living systems and their chance to function as novel biological active compounds. Therefore, development of new synthetic method of heterocyclic compounds bearing phosphorus atom is crucial. We foresee that the phosphacoumarin, which may be recognized as a phosphorus-containing analog of coumarin, would have pharmacological activities similar to those of coumarins described. As a consequence, we were attracted in expanding an efficient procedure for the synthesis of a number of phosphacoumarins with the purpose of making focused chemical libraries. We report an intramolecular hydroarylation of easily accessible aryl alkynylphosphonates catalyzed by gold/silver catalyst in the presence of TfOH in selective 6-*endo* mode, thus providing an effective and distinctive method for preparing phosphacoumarins having a range of functional groups.

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Rhodium-Catalyzed C-H Activation/Cyclization of Phosphonamide and Phosphinamide Group

박상준 서보람 신서현 손정유 김상혁 이필호*

강원대학교 화학과

Transition-metal-catalyzed C-H bond activations have been established to be a very efficient process for the formation of C-C and C-heteroatom bonds. In general, *ortho* C-H bond activation can be achieved by the application of a multitude of directing groups with the assitance of coordination of transition metals. We have recently interested in development of new phosphoryl-related directing groups in the C-H bond activations and its application to synthesis of phosphorus heterocyclic compounds. Although the oragnophosphorus compounds have been recognized as crucial compounds in the area of pharmaceutical and agricultural chemistry, their employment in transition-metal-catalyzed C-H bond activations has been barely studied. Herein, we report an efficient rhodium-catalyzed oxidative couplings *via* C-H activation and annulation using arylphosphonamides and arylphosphinamides under aerobic conditions, which produced benzazaphosphole 1-oxides and phosphaisoquinolin-1-oxides with high selectivity, a wide substrate scope and an excellent functional group tolerance.

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Direct C-3 Alkenylation of Phosphachromones through Palladium-Catalyzed C-H Activation

강동진 신서현 김철의 서보람 이필호*

강원대학교 화학과

Organophosphorus compounds have been received broad attention owing to their omnipresence in living organisms and their possibility to act as novel pharmaceuticals. Because there is a prominent likeness in chemical and biological property between the carbon and the corresponding phosphorus compounds, we envision that the phosphachromone which is phosphorus analog of chromone would have chemical, biological, and medicinal properties similar to chromone. Furthermore, we have been interested in developing an efficient synthetic method of a wide range of phosphachromones possessing a functionalized alkenyl moiety at the C-3 position with the purpose of making focused chemical libraries. However, there are no synthetic examples of C-3 alkenylated phosphachromone. Stimulated by C-H activation using cyclic enaminone, chromone, and phosphoryl-related directing groups, we imagined that the C-H activation method with phosphachromones would act as an effective route for the C-3-functionalization of phosphachromones. In this paper, we report new synthetic method for an efficient C-3-alkenylation of phosphachromones *via* Pd-catalyzed oxidative C-H functionalization under aerobic conditions.

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Synthesis of Benzoxaphosphole 1- and 2-Oxides through Palladium-Catalyzed C(sp^2 and sp^3)-H Activation/C-O Bond Formation

엄다한 김예린 최원석 서보람 이필호*

강원대학교 화학과

C-H activation catalyzed by transition metals has been recognized as a challenging objective in organic synthesis since unactivated C(sp^2)-H and C(sp^3)?H bonds are omnipresent in organic compounds. we have recently been interested in the development of novel phosphoryl-related directing groups in C-H activations and application to the synthesis of P-heterocyclic compounds due to a remarkable similarity in reactivity and bioactivity between the carbon species and their phosphorus counterparts. oragnophosphorus compounds have been identified as important compounds in the field of medicinal, material, and agricultural chemistry. An efficient synthetic method of benzoxaphosphole 1- and 2-oxides is reported from phosphonic and phosphinic acids without prefunctionalization through a Pd-catalyzed C(sp^2 and sp^3)?H activation/C-O bond formation under aerobic conditions.

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Synthesis and Electroluminescent Properties of Blue Emitters Based on 1,2,4-triphenyltriphenylene Derivatives for Organic light-emitting diodes

박수나 김영석 윤승수*

성균관대학교 화학과

In this study, we have synthesized blue emitters based on 1,2,4-triphenyltriphenylene groups using Diels?Alder reaction and their electroluminescent properties were investigated. Multilayered OLEDs were fabricated by using the compounds as emitting materials. The device structure was ITO / NPB (50nm) / emitting materials (30nm) / Bphen (30nm) / Liq /Al. In particular, a device showed efficient blue electroluminescent properties with luminous, power, external quantum efficiency and CIE coordinates of 1.11 cd/A, 0.51 lm/W, 1.15 % at 20 mA/cm2 and (0.16, 0.11) at 7V, respectively.

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ICl-Mediated Intramolecular Twofold Iodoarylation of Diynes and Diynyl Diethers and Amines: Synthesis of Bis(2*H*-hydronaphthalene and chromene) and 2*H*-Quinoline Bearing an Alkenyl Iodide Moiety

모준태 최원석 민지애 김철의 엄다한 김성홍[1] 이필호*

강원대학교 화학과 [1]한국기초과학지원연구원 대구분소

Electrophilic intramolecular twofold iodoarylation was developed from the reaction of diynes and diynyl diethers and amines with iodine monochloride under mild conditions, which produced bis(2*H*-hydronaphthalene and chromene) and 2*H*-quinoline bearing an alkenyl iodide moiety in good to excellent yields. These compounds underwent Pd-catalyzed cross-coupling reactions with arylboronic acid and indium tris(arylthiolate) to produce the functionalized styrene derivatives.

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Novel blue organic-light emitting materials based on 9,10-diphenylanthracene containing 9*H*-carbazole or 7*H*-benzo[c]carbazole group

이슬비 이현우 윤승수*

성균관대학교 화학과

Anthracene derivatives have been extensively studied as blue emitting materials in OLEDs due to their excellent photoluminescence and electroluminescence properties. In this study, a series of anthracene backbone with carbarzole derivatives was synthesized by a Buchwald reaction. To explore EL performances of these materials, we have fabricated blue OLEDs with the following device structure: ITO/2-TNATA (60 nm)/NPB (20 nm)/ αβ-ADN:Blue dopant materials (30 nm)/DNAB (30 nm)/Liq/Al. Among those, a device exhibited a maximum luminance of 10310 cd/m^2, a maximum luminous efficiency of 4.63 cd/A, power efficiency of 1.95 lm/W, an external quantum efficiency of 3.42%, and CIEx,y coordinates of (0.15, 0.17) at 20 mA/cm^2, respectively. In conclusion, these results demonstrate that anthracene as a molecular backbone with carbarzole derivatives as blue host materials would perform the excellent properties for OLED applications.

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Palladium-Catalyzed Decarboxylative C-H Alkynylation of Benzoxazoles with α,β-Ynoic Acids

강동진 유은정 조승윤 이필호*

강원대학교 화학과

Oxazoles are one of the most attractive heterocycles, especially in the pharmaceutical industry, the functionalization of oxazoles at a desired position has been extensively studied. The reactivity of electron deficient alkynes is barely sufficient to react with heterocyclic compounds under the reaction conditions. To overcome those difficulties, metal-catalyzed alkynylations of oxazoles with terminal alkyne surrogates, such as bromoalkynes or gem-dihaloalkenes, have recently been developed. Palladium-catalyzed decarboxylative C-H alkynylation of benzoxazoles with α,β-ynoic acids was achieved for the first time. This straightforward method was found to be synthetically effective without strong base under air.

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Synthesis 1,4-Di(1-pyrenyl)benzene based on pyrene derivatives for Organic light-emitting diodes

김찬우 김좌진 윤승수*

성균관대학교 화학과

In this study, we have synthesized four blue emitters based on pyrene end-capped groups by Suzuki coupling reactions. To explore EL performances of these materials, we were fabricated in the device structure in following sequence: ITO/NPB (50nm)/ Blue emitting materials / Alq_3 (15nm)/Liq (2.0nm)/Al (100nm). Among these, emitter A shows the maximum luminance of 11840 cd/m^2 at 12 V, the luminous efficiency of 4.04 cd/A at 500 cd/m^2, power efficiency of 1.99 lm/W at 500 cd/m^2 and the quantum efficiency of 2.49% at 500 cd/m^2 and CIEx,y coordinates of (0.17, 0.24) at cd/m^2.

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Optimization of the reaction conditions in the arylation step of carbazole type light emitting compound synthesis

Mohammed Samir* **Mahmoud Gamal Eldin*** **Mohammed I. El-Gamal[1,*]** **오창현[2,*]**

과학기술연합대학원대학교(UST) Biomolecular science [1]한국과학기술연구원(KIST) 생체재료연구단, Department of Medicinal Chemistry, Faculty of Pharmacy, Mansoura University, Mansoura 35516, Egypt [2]한국과학기술연구원(KIST) 바이오소재연구센터

Many carbazole compounds are employed in organic light-emitting diodes (OLEDs) either as host material for triplet emitters or as fluorescent emitter compounds. The majority of carbazole compounds used are arylated compounds. In this study, several attempts were done in order to obtain the optimal conditions for arylation of carbazole compounds. Solvent, base, time, and catalyst type and ratio were studied in order to get more feasible and industrial method for the synthesis of such compounds.

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Effect of the position based on a pyrene core for fluorescence materials

강현미 신환규 박종욱*

가톨릭대학교 화학과

OLED 의 발광체로 쓰이는 pyrene 을 기반으로 electron density 의 차이에 따른 색상의 변화와 OLED device 효율의 변화를 알아보았다. Pyrene 의 electron rich position 에 side 를 붙인 1,6-DSPy 와 electron poor position 에 side 를 붙인 2,7-DSPy 의 optical properties 를 비교해 보았을 때 solution 과 film UV spectra 에서 1,6-DSPy 가 2,7-DSPy 보다 red shift 하였고, PL spectra 에서도 1,6-DSPy 가 상대적으로 red shift 한 maximum emission peak 을 가졌다. OLED device 에서 2,7-DSPy 는 maximum EL emission 이 475nm, 492nm 이고 CIE coordinates 는 (0.179, 0.368)이며, external quantum efficiency 가 1.79%의 특성을 나타내었다. OLED device 에서 1,6-DSPy 는 maximum EL emission 이 535nm, 565nm 이고 CIE coordinates 는 (0.436, 0.549)이며, external quantum efficiency 가 2.08%의 특성을 나타내어 device 효율면에서는 1,6-DSPy 가 상대적으로 우수한 효율을 나타내는 것을 확인하였다.

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Calix[4]tetrahydrothiophenopyrrole: Control of Cation Binding Site via Peripheral Modification of Calix[4]pyrrole

이창희* **SAHAINDRAJIT** 유소은

강원대학교 화학과

Calix[4]pyrroles which are fused with tetrahydrothiophene have been synthesized and characterized. The ion binding study of the synthesized hosts displayed very interesting properties. The deep cavity, cation binding pocket which was created by anion binding shows different selectivity depending on the nature of applied cations. For example, the cone conformation resulting upon the pre-complexation with fluoride anion, forms stable ion-pair complex with cesium cation. The cesium cation is thought to be bound to the deep inside the cavity by cation-pi interaction. On the other hand, the mercury(II) ion form stable donor-acceptor complex with the sulfur atom. The ion binding studies confirmed that the synthesized receptors form stable complexes with various metal salts in organic media. The binding affinities and spectroscopic changes upon ion binding will be presented

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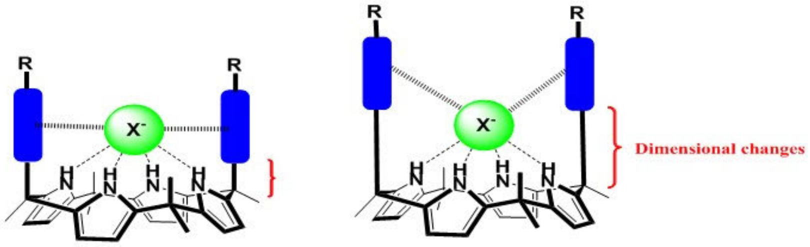
meso-Substituent Effect on the Anion Recognition Properties of Calix[4]pyrroles

이창희* <u>하민지</u> 이정태[1]

강원대학교 화학과 [1]한림대학교 화학과

Series of calix[4]pyrroles bearing meso-aryl group at diametrically crossing meso-positions have been synthesized and characterized. The guest binding pocket created by the two meso-aryl groups and four pyrrole N-Hs are expected to recognize anionic guests through hydrogen bonding and anion-pi interaction. The size discrimination is also expected due to the limited dimension of the binding pocket. The combined interactions is expected to exhibit enhanced affinity and selectivity toward anionic guests. The anion binding studies revealed that all the synthesized receptors form stable complex with various anions in acetonitrile. The cis-5,15-bis(meso-phenylehtynyl)-substututed calix[4]pyrrole showed enhanced binding affinities than the cooresponding cis-5,15-bis(meso-phenyl)-substituted calix[4]pyrrole. This results indicated that the ethynyl spacer is necessary for the effective anion-pi interaction. Cooperative interactions of hydrogen bonding and anion-pi interaction was operating and playing the key role on the enhanced binding affinity. The receptors synthesized here would be good model systems for dimensional probes for the anion binding and designing quest selective anion receptors


R
R
X⁻
R
R
X⁻
Dimensional changes

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Unprecedented non-aromatic, confomationally locked dibenzohexaphyrin analogs carrying multiple meso-exocyclic double bonds

이창희* 황선아 김진경

강원대학교 화학과

The chemistry of the expanded porphyrins has been one of the important topics in conjunction with in-depth understanding of the macroaromaticity and their unique spectroscopic properties. One of the most interesting aspects of expanded porphyrins are their topological features. So called, ‘figure-eight’ conformation of octaphyrin inherently induce chirality of the systems and often shows intriguing aspects of the aromaticity of the system. The expanded porphyrins display unique structural features and often show considerably red-shifted absorption maximum relative to those of classical porphyrins. As part of the continuing efforts to understand the interplay between the electronic features of the porphyrins and aromaticity, we have been interested in the development of new meso-alkylidenyl porphyrin analogues Acid-catalysed, ‘3+3’ condensation of m-bispyrryl benzene derivatives with acetone afforded new non-aromatic macrocycles that can be converted to meso-alkylidenyl dibenzohexaphyrins by DDQ oxidation carrying four exocyclic double bonds at meso-positions. The non-aromatic porphyrin analogs reported here are optically inactive in spite of the presence of multiple stereogenic centers. However, most compounds obviously adopt chiral conformation at least in solid state.

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Conformational and structural characteristics of meso-alkylidenyl benzipentaphyrins

이창희* 황선아 김보람

강원대학교 화학과

The novel meso-alkylidenyl porphyrins are non-aromatic and conformationaly flexible macrocycles. Most of the compounds displays interesting site-selective protonation depending on the number of core-hydrogen upon treatment with acid. As a part of our continuing efforts for the construction of the new expanded version of the congeneric macrocycles, we here report the synthesis, characterization and conformational characteristics of meso-alkylidenyl benzipentaphyrins. The synthesis is accomplished by a typical ‘3+1’ type of the mixed-condensation. The structural characterization indicates that the compounds contain two exocyclic carbon-carbon double bonds at meso-positions and different number of inverted pyrroles. The p-benzipentaphyrin show asymmetric nature in proton NMR spectra, indicating some of the pyrrole rings are inverted conformation. The structural characteristics and protonation selectivity upon addition of acid will be extensively discussed.

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Highly selective fluorescence turn-on probe for biothiols

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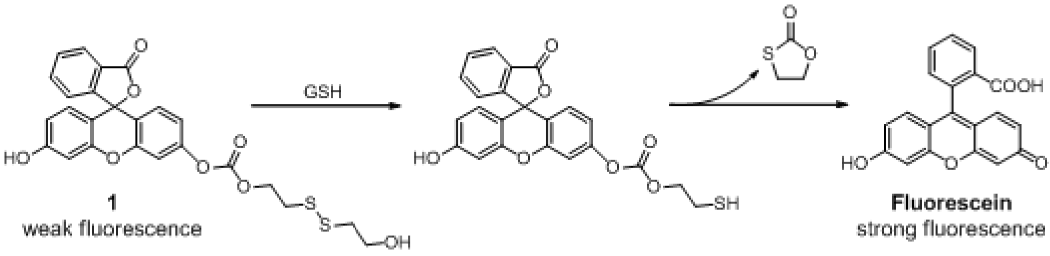
한국외국어대학교 화학과 [1]한국외국어대학교 자연과학대학 화학과

Biothiols such as cysteine (Cys), homocysteine (Hcy), and glutathione (GSH) play important roles in such processes as redox homeostasis [1] and cellular growth [2] in a biological system. An abnormal level of biothiols is an indicator of human diseases like cancer and AIDS. [3] Therefore, we report a designed fluoresceinylcarbonate-based fluorescent probe for the rapid detection of biothiols. The probe has shown a rapid and sensitive response to biothiol, glutathione over other various amino acids through the disulfide bond cleavage and the subsequent intramolecular cyclization. When glutathione was added, fluorescence of probe was significantly enhanced which was observable by the naked eye and in living cells. [4]References[1]. (a) Dalton, T. P.; Shertzer, H. G.; Puga, A. *Annu. Rev. Pharmacol. Toxicol.* 1999, *39*, 67. (b) Mathews, C. K.; van Holde, K. E.; Ahern, K. G. *Biochemistry*; Addison-Wesley Publishing Co.: San Francisco, 2000. [2]. (a) Wood, Z. A.; Schroeder, E.; Harris, J. R.; Poole, L. B. *Trans-Biochem. Sci.* 2003, *28*, 32. (b) Carmel, R.; Jacobsen, D.W. *Homocysteine in Health and Disease*; Cambridge University Press: Cambridge, 2001.[3]. (a) Townsend, D. M.; Tew, K. D.; Tapiero, H. *Biomed. Pharmacother*. 2003, *57*, 145. (b) Herzenberg, L. A.; De Rosa, S. C.; Dubs, J. G.; Roederer, M.; Anderson, M. T.; Ela, S. W.; Deresinski, S. C.; Herzenberg, L. A. *Proc. Natl. Acad. Sci. U.S.A.* 1997, *94*, 1967. [4] Hong, K.-H.; Kim, D. I.; Kwon, H.; Kim, H.-J. *RSC Adv*. 2014, *4*, 978


GSH
HO
O
O
O
O
O
S
S
OH
1
weak fluorescence
HO
O
O
O
O
O
SH
S
O
O
COOH
HO
O
O
Fluorescein
strong fluorescence

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발표종류: 포스터, 발표일시: 수 16:00~19:00

Rapid visual detection of cyanide by azo dye-based probe

나상윤 김해조[1,*]

한국외국어대학교 화학과 [1]한국외국어대학교 자연과학대학 화학과

Cyanide ion is one of the most toxic anions and is deadly to human health [1]. But it is still widely used in various industrial processes such as gold mining, electroplating, metallurgy, chemical products [2]. Therefore, it is highly desirable to develop rapid and simple sensing systems for cyanide. Therefore, we report a designed probe (1) for cyanide that was prepared through the oxime formation. Cyanide ion attack toward the oxime function of probe (1) and then followed by fast proton transfer of oxime hydrogen to the developing alkoxide anion of probe (1). So azo dye-based probe (1) displays a violet color upon binding to the toxic cyanide with rapid reaction.References[1]. Baskin, S. I.; Brewer, T. G. *In Medical Aspects of Chemical and Biological Warfare*; Sidell, F., Takafuji, E. T., Franz, D. R., Eds.; TMM Publications: Washington, DC, 1997; pp 271?286. [2]. Koenig, R.; *Science*, 2000, *287*, 1737

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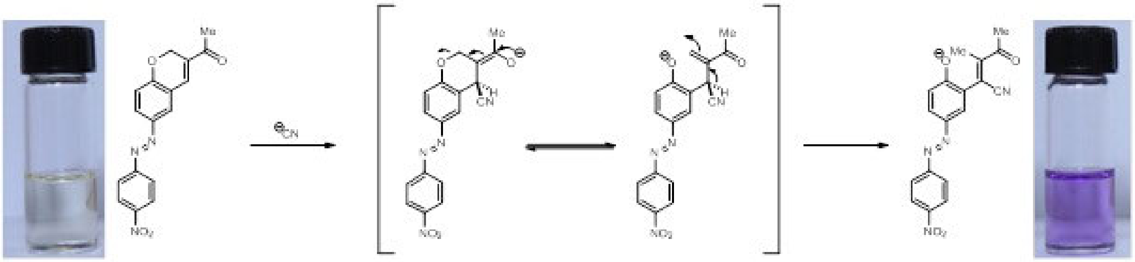
Azo dye-based Latent Colorimetric Chemodosimeter for the Selective Detection of Cyanides in Aqueous Buffer

박석안 김해조*

한국외국어대학교 자연과학대학 화학과

Cyanide is hazardous chemical that damages by absorption through the lungs, gastrointestinal tract, and skin, and can kill mammals upon binding to a heme unit. [1] Humans may be exposed to cyanides from dietary, industrial, environmental, and other sources. Consequently, there is of considerable interest in detecting the presence of the toxic cyanides by using chemosensors. [2] There are, however, a few chemical probes [3] that are operating in water and show both the colorimetric and fluorescence changes upon the complexation of cyanide anions. [4] We prepared a latent colorimetric probe (1) for cyanide. Upon the addition of cyanides, probe 1 underwent a ring opening reaction through the Michael addition of cyanide and a subsequent [1,3]-sigmatropic rearrangement reaction gave rise to a stable free phenol group, whose signal was transduced into the azo dye unit to afford dramatic color changes. The chemodosimeter exhibited a highly selective and colorimetric response to cyanide ions over other anions. The dramatic color changes of 1 allowed us to detect toxic cyanide anions even by the naked eye in aqueous solution.



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Syntheses of Fused Pyrrole-2-carboxylates via Cu-catalyzed one-pot HWE-reaction/N-arylation

임환정* 최지혜[1] 이진용[2] 신승훈[1,*]

한국화학연구원 의약화학연구센터 [1]한양대학교 화학과 [2]충남대학교 신약전문대학원

Synthesis of various fused pyrrole-2-carboxylates was accomplished via Cu-catalyzed one-pot HWE-reaction/N-arylation at room temperature. This new method gave various fused pyrrole-2-carboxylates in good to excellent yields under exceptionally mild reaction conditions using commercially available starting materials.

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DDQ-Mediated Indole Synthesis

장영호 조윤형 윤소원*

한양대학교 화학과

2,3-Dichloro-5,6-dicyano-1,4-benzoquinone (DDQ) is the chemical reagent as an oxidant which is useful for the dehydrogenation of alcohols, phenols, oxidative couplings, and cyclization reactions in organic chemistry. Recently, we have developed a DDQ-mediated intramolecular oxidative cyclization reaction of *N*-Ts-2-styrylanilines to afford a variety of indoles in high yields.

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Pd-Catalyzed Oxidative Cyclization for Indole Synthesis

이소라 윤소원*

한양대학교 화학과

A new Pd-catalyzed oxidative cyclization reaction has been developed for the synthesis of indoles. Depending on the reaction conditions, different types of product could be obtained. Most substrates with various *N*-protecting groups including sulfonyl showed similarly moderate reactivity and gave good chemical yields. Investigations to improve the reaction efficiency and selectivity as well as to expand the scope of this reaction have been performed.

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Unusual Fluorescence Response Pattern Guided Bio-thiols Identification and Cellular Imaging of GSH varition in Carcinoma Cells, Tissues, and Bloods

임문수 이재홍 장주희 이윤학 신원섭 김종승*

고려대학교 화학과

A novel ratiometric fluorescent probe 1 was developed for detection of thiol-containing amino acids. This probe successfully discriminates between human carcinoma and normal cells by detecting intracellular thiol levels in living cells. The ability of the probe to identify growing tumors by measuring GSH in the tissues as well as in the fresh blood of tumor xenograft mice, suggests that it represents a promising prognostic and diagnostic marker, with extensive and simple potential clinical applications.

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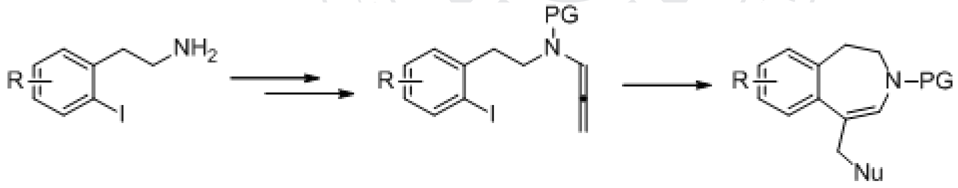
Synthetic study of derivatives of benzazepine structure from palladium-catalysed cyclization of alleneamide

김홍택 김건철*

충남대학교 화학과

Various derivatives of benzazepine structure were isolated from the plants of the Chilean Berberis species. Their unique structure feature, five- and seven-membered rings fused with aromatic moiety has drawn the synthetic interest of many group. We have studied a cyclization of alleneamide derivatives for the formation 8-membered benzazepine ring using palladium catalyst.



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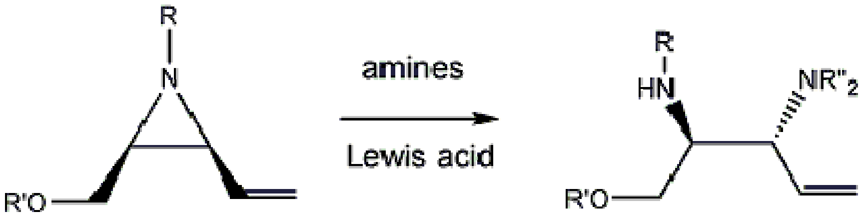
Synthesis of vicinal diamines by ring-opening of 3-substituted-2-vinylaziridines

강한영* <u>강온유</u>

충북대학교 화학과

Because vicinal diamine moiety is an important structural part in many biologically active molecules such as anti-cancer agents and anti-influenza drugs, efficient methods for the preparation of 1,2-diamines have been a subject for the intensive studies. Vicinal diamines have also been used in chiral auxiliaries and chiral ligands. One of the efficient methods for the stereoselective synthesis of the vicinal diamines has been the nucleophilic ring-opening of properly substituted chiral aziridines. We have recently investigated the regio- and stereoselective ring-opening of cis-3-substituted-2-vinylaziridines. Encouraged by the easy preparation of enantiomerically pure chiral aziridines and selectivity in ring-opening of vinylaziridines, we have decided to investigate the ring-opening of cis-3-substituted-2-vinylaziridines by nitrogen-containing nucleophiles leading to vicinal diamines. Aliphatic and aromatic amines in the presence of a Lewis acid have been successfully employed in the regio- and stereoselective ring-opening of the aziridines. Details of the investigation will be reported.



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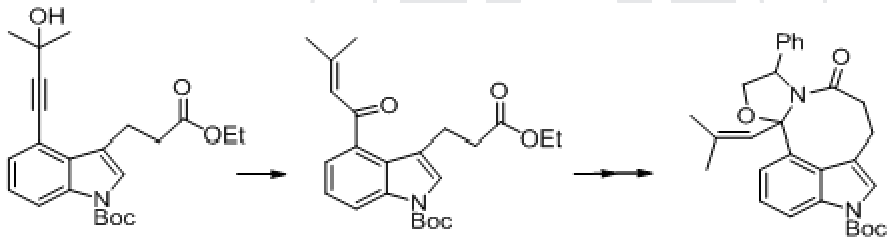
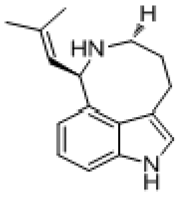
Synthetic study of an azepinoindole alkaloid, aurantioclavine

이수진 김건철*

충남대학교 화학과

Aurantioclavine, one of the representative ergot alkaloid, was isolated from Penicillium aurantiovirens in 1981. In this study a azepinoindole derivative has been synthesized by indole synthesis, meyer-schuster rearrangement and meyer's methodology. Using this methods, we are going to synthesize aurantioclavine.





Aurantioclavine

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Dansy-thiazole conjugate as divalent copper sensor

김보연 안미란 김홍석*

경북대학교 응용화학과

The developments of turn-on fluorescent probes have attracted attention. Previously, the synthesis and Zn^{2+} or Al^{3+} sensing properties of several thiazole based chemosensors were reported. A new highly selective fluorescent dansyl-thiazole conjugate was synthesized and investigated for the quantification of copper and iodide anions in acetonitrile.

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Gallium-selective ‘turn-on’ fluorescent chemosensor

김보연 안미란 김홍석*

경북대학교 응용화학과

Ga (III) is known to be highly toxic and cause carcinogenesis in animals and humans. Symptoms of acute poisoning including gastrointestinal discomfort, vomiting, coma, and sometimes death usually occur within 30 min of ingestion of gallium arsenide (GaAs), whereas the consequences of chronic poisoning including anemia, leucopenia, skin cancer, and other internal cancers are much more insidious. Therefore its determination is very crucial for health and economic purposes. Three new highly selective turn on fluorescent chemosensors for gallium ions were synthesized and investigated.

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Synthesis and OLED Property of Cyclometalated Platinum(Ⅱ) Complexes

도희진 김영준*

충남대학교 화학과

Cyclometalated metal complexes are among the most efficient phosphorescent materials and have been widely explored for use in chemical sensors and organic light-emitting diodes(OLEDs). In particular, the efficient phosphorescence of cyclometalated platinum(Ⅱ) β-diketonates has led to many applications in biological imaging, nonlinear optics, oxygen sensing, and most notably electroluminescent devices. Substituted phenyl imidazoles were prepared by the reaction of the substituted phenylaniline, glyoxal, NH_4Cl and formaldehyde, in the presence of H_3PO_4 in THF and Methanol. These compounds were methylated and cyclometalated platinium complexes were obtained after the reaction with the silver oxide, $[PtMe_2(SMe_2)]_2$ and β-dikotones. The products were characterized by ^1H- and ^{13}C-NMR spectroscopy. UV-Vis absorptions maxima of these compounds occur at 320nm and PL spectra are shown at 470nm ～ 480nm. We will also report OLED property including EL spectra.

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Practical Multigram Synthesis of Spirobisindane Derivatives and Its Application of Heterocycle Syntheses

최지수 이기정* 이영무[1,*]

한양대학교 화학공학과 [1]한양대학교 화학공학

Polymers of intrinsic microporosity containing 1,1'-spirobisindane building blocks as subunits are very attractive for the construction of gas separation membranes. This work discloses an easy-to-handle and chromatography-free synthetic method that can furnish the valuable monomer 3,3,3',3'-tetramethyl-1,1'-spirobisindane-5,5'-diamino-6,6'-diol in multigram quantities and its application of new heterocycle syntheses.

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Total Synthesis of Phorbaketals

이재연 이희윤*

한국과학기술원(KAIST) 화학과

Phorbaketal A and derivatives were isolated by Rho et al. in 20091) from the Korean marine sponge Phorbas sp. and it exhibits cytotoxicity against human colorectal, hepatoma, and lung cancer cell lines. Phorbaketal A possesses an unprecedented structure that is novel spiro[5,5]ketal fused to a hydrobenzopyran ring. Since Phorbaketals has unprecedented structural features through an interesting biosynthetic pathway as well as interesting biological activities, we became interested in the total synthesis of these natural products.We envisioned that the total synthesis of phorbaketal A can be achieved through Au mediated cyclization reaction of the precursor readily prepared from carvone and geranial. The key step of this synthesis is Au(I) catalyzed intramolecular cyclization of diol and internal alkyne. The diol-alkyne key intermediate was synthesized by coupling of two fragments derived from (R)-Carvone and Geraniol respectively, using Cu(I) catalyzed reaction.Recently new Phorbaketal derivatives are isolated from the same marine sp.2) and another Korean marine sponge of the genus Monanchora3). These all different Phorbaketals are synthesized from Phorbaketal A for the first time. References1.Rho, J.-R.; Hwang, B. S.; Sim, C. J.; Joung, S.; Lee, H.-Y.; Kim, H.-J. Org. Lett. 2009, 11(24), 5590-5593.2.Unpublished.3.Wang, W.; Mun, B.; Lee Y.; Reddy, M.V.; Park, Y.; Lee, J.; Kim, H.; Hahn, D.; Chin, J.; Ekins, M.; Nam, S.-J.; Kang, H. J. Nat.Prod. 2013, 76, 170-177

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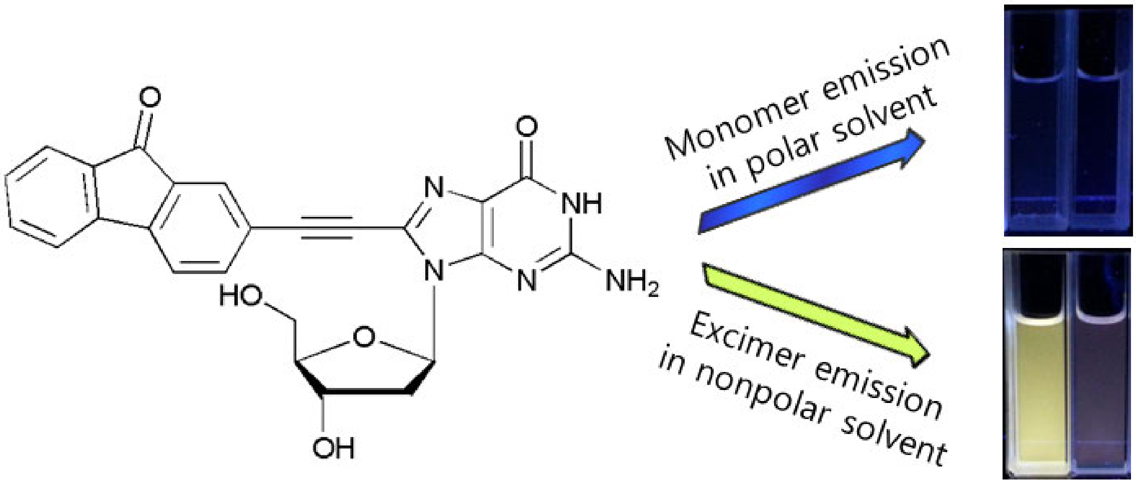
2´-Deoxyguanosine labeled with fluorenone unit for an excimer probe

김민주 황길태*

경북대학교 화학과

Fluorescent nucleosides that are sensitive to their physical environment, including the presence of other molecular species in solution, resulting in specific changes in their fluorescence properties, are powerful tools for investigating nucleic acid structures, recognizing single nucleotide polymorphisms, and studying enzymatic processes involving DNA. In this study we prepared two fluorescent nucleosides, G^{FL} and G^{FO}, comprising 2´-deoxyguanosine units covalently bound to 2-ethynylfluorene and 2-ethynyl-9-fluorenone moieties, respectively. The photophysical properties (fluorescence emission shifts and emission intensities) of these fluorescent nucleosides are solvent-dependent. Most notably, G^{FO}, which bears a guanine nucleobase as its electron-donating group, displays an excimer emission in nonpolar solvents; accordingly, we used excimer emission titration to determine the binding constants for the interactions between G^{FO} and nucleobases.



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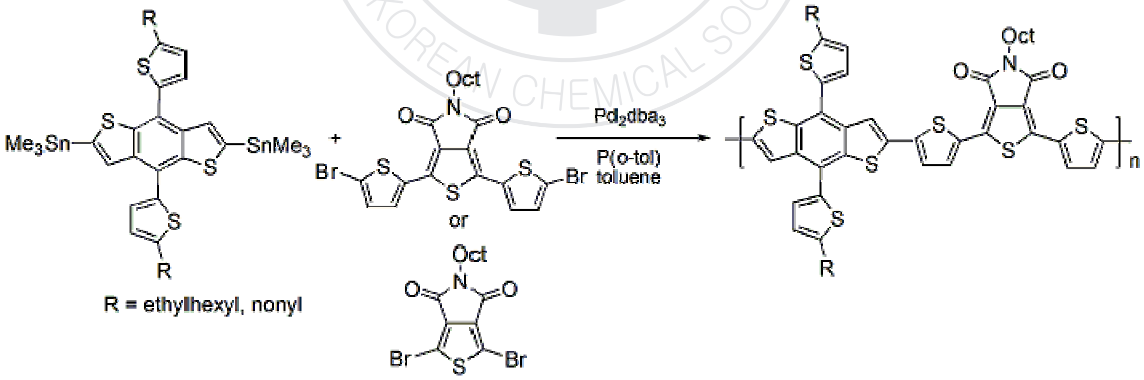
Synthesis and characterization of two-dimensional BDT-TPD conjugated copolymers for polymer solar cells

정규관* 홍남정[1]

전북대학교 과학교육학부 [1]전북대학교 사범대학화학교육과

Two-dimensional structured benzo[1,2-b;4,5-b']dithiophene (BDT) derivatives functionalized with branched or linear alkyl group were synthesized and copolymerized with N-alkylthieno[3,4-c]pyrrolo-4,6-dione. Three different copolymers depending on alkyl groups were synthesized and characterized by NMR, GPC, DSC, and UV-vis, cyclovoltammetry. Structure-property relationship of the polymers were investigated.



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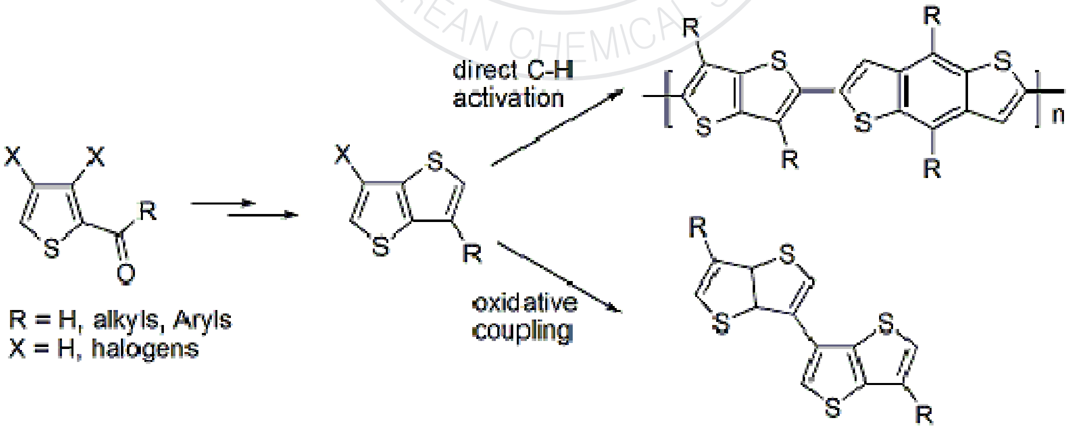
Synthesis and characterization of alkylthieno[3,2-b]thiophene derivatives as a building block for D-A conjugated polymers

정규관* 이명지[1]

전북대학교 과학교육학부 [1]전북대학교 화학교육과

Starting from 3-bromothiophene or 3,4-dibromothiophene, a variety of alkylthieno[3,2-b]thiophene derivatives were synthesized and fully characterized. Several steps of manipulations of those compounds afforded useful donor subunits for D-A conjugated polymers. Polymerization through direct C-H activation employing these compounds were attempted and evaluated. These compounds were also subjected to dimerization via oxidative coupling in order to get extended conjugated oligomers for OFET and results are discussed.



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A push-pull benzothiazole based fluorescent probe for cyanide and its application to paper based sensor

이동남 홍종인*

서울대학교 화학부

Highly toxic cyanide compounds are commonly occurring chemicals found in surface water not only from industrial waste but also from biological sources. In this study, we monitored on colorimetric and fluorogenic response of synthetic probe 1 toward cyanide. The designed synthetic probe has a strong push-pull electronic effect, and consequently it provides light absorption and emission properties at longer wavelength. After encountering with cyanide, the push-pull system of the probe turned out to be destroyed in the broken pre-exited pi-conjugation, resulting in changes of various photophysical properties. Nowadays, paper-based test strips are considered to open new application fields in rapid and easy to use for point-of-care testing areas including clinical diagnosis, food quality control and environmental monitoring. In this regard, the probe was imposed onto paper based sensor for cyanide field test. Incorporating the probe with digital ink jet wax printing techniques, simple paper-based devices were easily established. Quantitative analysis with the fabricated paper sensor upon increasing cyanide administration showed different fluorescence intensities with linear detection range up to 30 mM, which was easily digitized imposing into Adobe Photoshop software, whereas no response to other competitive analytes such as SH-, HPO42-, OAc-, N3-, F-, Cl-, Br-.

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Coumarin-Derived Cys-Selective Fluorescence Probes Using Molecular modulation

정효성 구세영 김원영 강철훈[1] 김종승[*]

고려대학교 화학과 [1]경희대학교 동서의학대학원

A series of coumarins, each bearing a double bond conjugated benzoate unit that can undergo a Michael-type reaction with thiol-containing compounds, is presented. The only difference among the coumarins is the position of a carboxyl group on its benzene ring moiety near the double-bond conjugated coumarin. Their selectivity for Cys, GSH, and Hcy as well as the associated fluorogenic mechanism were illustrated by fluorescence spectroscopy, and kinetic studies. All probes prefer Cys over GSH in the reaction from 48.6 to 111-fold as demonstrated in a second order kinetics. The high selectivity of probes to Cys might be achieved since the *ortho* carboxyl group on its benzene ring prefers a less negatively charged nucleophile. During intracellular Cys detection using this probe, a possible interference by a large amount of GSH in the HepG2 cells was evaluated. The cells were treated with L-buthionine sulfoximine (BSO), an inhibitor of *r*-glutamylcysteine synthetase, providing an experimental condition where the cells could not synthesize GSH from Cys or other species. Then, the fluorescence intensity of probe in HepG2 cells under BSO-H_2O_2 treatment was strongly enhanced by *N*-acetylcysteine (NAC), a precursor of Cys, implicating that the fluorescence signal from the cells is mainly associated with changes in intracellular [Cys] rather than that in intracellular [GSH].

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발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis of Multivalent Nucleating Ligands for Controlling Protein Crystallization

김희권* 권영도[1]

전북대학교 의학전문대학원/핵의학교실 [1]한국기술교육대학교 응용화학공학과

Since nucleation is the first step in the crystallization process, the development of a general method to control protein nucleation could help to reduce the bottleneck in the protein crystallization process. We have developed a small library of highly symmetric, conformationally-restricted, water-soluble multivalent nitrilotriacetic acid ligands that have been designed to bind proteins bearing polyhistidine tags in a symmetry-guided manner in the presence of Ni2+. These reagents seek to control protein:ligand speciation and promote self-assembly of the protein:ligand complexes in a manner that provokes his-protein crystal nucleation and growth. Several lines of evidence suggest that these materials achieve these design goals. Size exclusion chromatography analysis of using histidine-tagged green fluorescent protein (his-GFP) as a model confirmed the presence of higher molecular weight species in solution; however, due to limitations of the technique only average molecular masses of the major species formed could be determined. Higher resolution studies utilizing analytical ultracentrifugation confirmed the presence of dimers, trimers, and tetramers of his-GFP when using a 2-fold, 3-fold, or 4-fold ligand, respectively, as well as higher molecular weight oligomers that presumably arise from ligand-guided self-assembly of these species. Transmission electron microscopy analysis of the complexes reveals the formation of elongated needle-like structures, similar to the preferred crystal morphology of GFP. We infer from these findings that protein speciation can be controlled, and crystal nucleation induced, using highly symmetric multivalent NTA chelating agents of this type.

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Synthesis of Novel Imaging Agent and Nanocarriers for Fibronectin Attachment Protein (FAP) as a Targeting Vector for Bladder Tumor Cells

김희권

전북대학교 의학전문대학원/핵의학교실

Bladder cancer is the fourth most common cancer in men and eleventh most common in women in the US. Because of high recurrence rate and long interval progression, secondary adjuvant therapies are needed. After the effectiveness of intravesical live Mycobacterium bovis bacillus Calmette-Guerin (BCG) for the treatment of superficial bladder tumors was reported, BCG now is the treatment of choice for superficial bladder cancer in spite of significant side effects of modality. Ratliff et al. reported that fibronectin attachment protein (FAP) mediates the attachment of the BCG bacterium to the urothelial surface via the extracellular matrix protein fibronectin. To enable mechanistic and therapeutic aims of these studies, novel Tris- nitrilotriacetic acid (NTA)-Alexa probes and NTA-PEG-lipids were prepared and tested for their ability to promote bladder cells internalization of his-tagged FAP. Novel, acid-sensitive, tunable, and bifunctional cross linkers based on phenyl substituted vinyl ether (PIVE) were developed for delivering drugs to bladder tumors. Content release rate via acid-catalyzed dePEGylation could be altered by controlling hydrolysis of the cross linker by the addition of electron donating and withdrawing groups onto a phenyl ring for efficient delivery of contents. The phenyl substituted vinyl ether linkers could be potential candidates for the formulation of acid-sensitive carriers able to delivery gene and drugs into bladder and other tumor cells.

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발표종류: 포스터, 발표일시: 수 16:00~19:00

First total synthesis of the prioline based on a stille coupling/aldol condensation

박경용 송하정 허정녕[1,*]

충남대학교 신약전문대학원 [1]한국화학연구원 의약화학연구센터

The oxindole ring system constitutes an important group of polycyclic compounds that is found in natural products include aristolactams, anhydrohapaloxindole A, and prioline. Among them, Prioline was isolated from the roots of a species of Salvia, a genus whose plants are used in Chinese folk medicine for the treatment of tonsillitis, pharyngitis, pulmonary tuberculosis, and bacillary dysentery.Herein, a new approach for the synthesis of prioline has been developed via a stille coupling/aldol condensation as a key step

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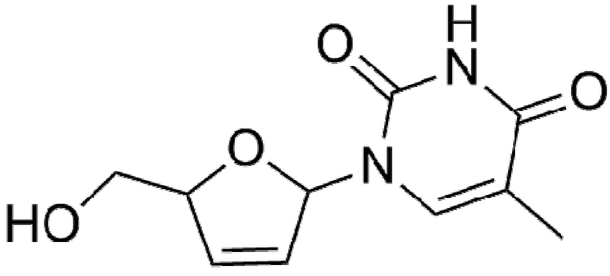
새로운 항 바이러스제의 개발을 위한 중간체의 합성(Synthesis of novel intermediates for new antiviral agents)

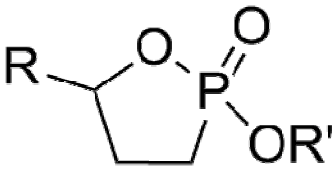
김태우 한용성 정강연*

강릉원주대학교 생명화학공학과

바이러스성 질환들은 현대인의 건강에 문제를 일으키는 큰 원인 중에 하나이다. 일반적으로 잘 알려진 바이러스성 질환들로 폐렴, 볼거리, 홍역, 독감, HIV 등이 있다. 그 중 HIV 는 인간 면역결핍 바이러스라고 하여 후천성 면역 결핍 증후군을 일으키는 바이러스이다. 이 바이러스에 감염되게 되면 신체의 면역세포인 CD4 양성 T-림프구가 파괴되어 면역력이 떨어지게 되고 그 결과 각종 감염성 질환과 종양이 발생하여 사망에 이르게 된다. 최근 이 HIV 의 전사과정을 막아 강력한 억제성을 갖는 뉴클레오사이드 유도체들이 개발되었고 이들 중 비라문, 3TC, AZT(d4T)를 병용할 때 최대 94%까지 박멸 가능한 연구 결과가 보고 되었다. 따라서 본 연구진이 개발한 인화학을 이용하여 d4T 와 유사한 구조를 가진 인을 포함한 중간체를 합성하고자 한다



d4T



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Construction and characterization of novel molecular architectures through coordination-driven self-assembly: rhomboid and overlapped double rhomboid

김점종 곽옥금[1] 박종근[1] 민길식[2,*] 윤용진[3,*]

한국전자통신연구원 IT부품산업기술연구부 [1]경상대학교 화학교육과 [2]경북대학교 사범대학 화학교육과 [3]경상대학교 화학과

Over the past few decades, coordination-driven self-assembly has been used to build two- and three-dimensional molecular architectures. Metal-directed self-assembly has been proven to be a powerful tool for the construction of well-defined coordination architectures with increasing structural diversity. This approach offers various opportunities for the preparation of nanoscopic supramolecular ensembles of predetermined shapes, sizes, and geometries. Many metallosupramolecules such as polygons, cages, and prisms have been reported. The well-defined structures formed by coordination-driven self-assembly can be applied for synthesis of metallosupramolecular dendrimers, encapsulation of guests, catalysts and sensors. These architectures were spontaneously generated by mixing designed building units (acceptor and donor) in a suitable solvent. The shapes of building blocks are determined by adjusting the angles between the bonding sites of individual components. Thus we have designed terpyridyl ligands with different nitrogen positions, in which interesting architectures such as rhomboid and overlapped double rhomboid can be obtained by combination with 2,9-bis[trans-Pt(PEt3)2(NO3)]phenanthrene. These supramolecular polygons containing free nitrogen atom can be potentially used for synthesis of new polyhedrons, molecular recognition, and encapsulation. To the best of our knowledge, the overlapped double rhomboid is new molecular architecture. Herein, we report the syntheses and structures of two terpyridine ligands, rhomboid, and overlapped double rhomboid via coordination-driven self-assembly.

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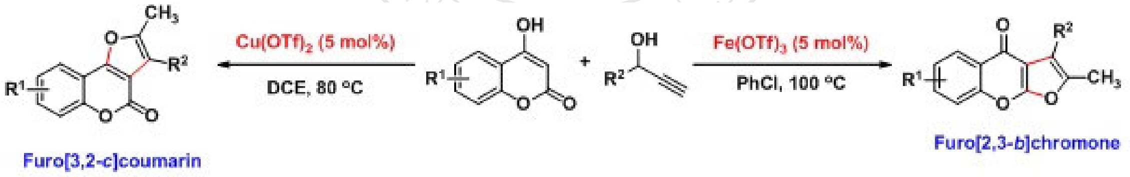
Selective synthesis of furo[3,2-*c*]coumarins and furo[2,3-*b*]chromones via tandem propargylation/alcohol-alkyne cyclization switched by different metals

김재현 이구연*

강원대학교 생명건강공학과

We described two tricyclic oxygen containing heterocycle synthesis, where an arene both an ancohol and an alkyne functionality underwent two distinct pathways catalyzed by different metal salts. Starting from 4-hydroxycoumarin and propargyl alcohol, furo[3,2-*c*]coumarins was accomplished by a Cu(II) salt, while furo[2,3-*b*]chromones could be accessed via a Fe(III) salts. This method provides a flexible and efficient route to substituted furocoumarins and furochromones, respectively.



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Syntheses of quinoxalines or dibenzo[a,c]phenazines from o-nitroanilines via indium-mediated heterocyclizations (Ⅱ)

고아라 배설희 이병민[1] 김병효[*]

광운대학교 화학과 [1]한국화학연구원 신화학연구단

Syntheses of quinoxaline or dibenzo[a,c]phenazine moiety-containing organic molecules have been considerable attention because of their biological activities or chemical futures. Indium is progressively applied to organic synthesis during the past two decades because it is environmentally favorable compared to other metals and it has low first ionization potential that is good enough for SET reaction.By applying indium-mediated reactions, we could develop new and efficient one-pot synthesis of nitrogen containing heterocycles, quinoxalines or dibenzo[a,c]phenazines, in this study. After the various reaction conditions examined, we found a proper reaction condition, i.e. 2-nitroanilines with indium in the presence of AcOH in MeOH and/or toluene. Thus, from a variety of o-nitroaniline derivatives with 9,10-phenanthrenequinone or 1,2-diketones such as 2,2’-thenil, 2,2’-pyridil, dibenzo[a,c]phenazines or quinoxalines were synthesized in moderate to excellent yields.

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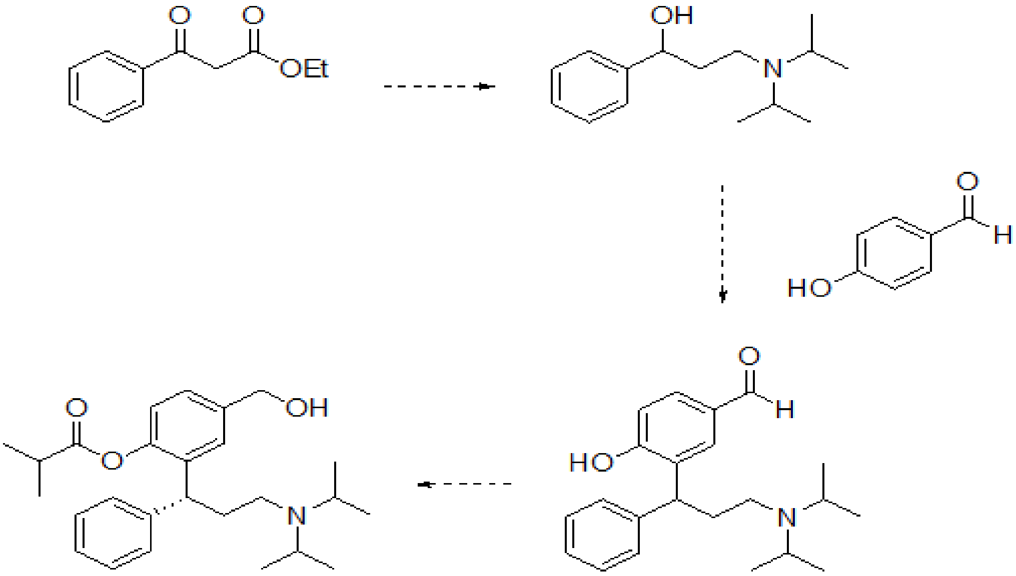
Development of an Efficient and Recyclable Gold Catalyst Supported on Thermosensitive Polymer and its application on A-3 Coupling in Water

shabbir saira 이영은[1] 이학준*

한양대학교 응용화학과 [1]한양대학교 바이오나노학과

Poly(NIPAM-co-4-VP) is capable of showing phase transition (PT) with temperature in hydrophilic solvents. Coordination of gold (III) with the Polymer results in a distinguishable combination of metal catalytic activity with the Polymer′s inverse solubility phenomenon. It catalyzes A-3 coupling reaction in water with excellent yields. As the Low Critical Solution Temperature (LCST) of Poly(NIPAM-co-4-VP) is 48˚C so it enabled us to optimize the reaction under quite mild conditions in aqueous medium. So, we developed a magnificent heterogeneous catalyst for A-3 coupling reaction in water. The catalyst is also efficient, recyclable and stable in air. It can tolerate a variety of substrates and we except that it can be employed for other gold catalyzed organic transformations too.



Fesoterodine

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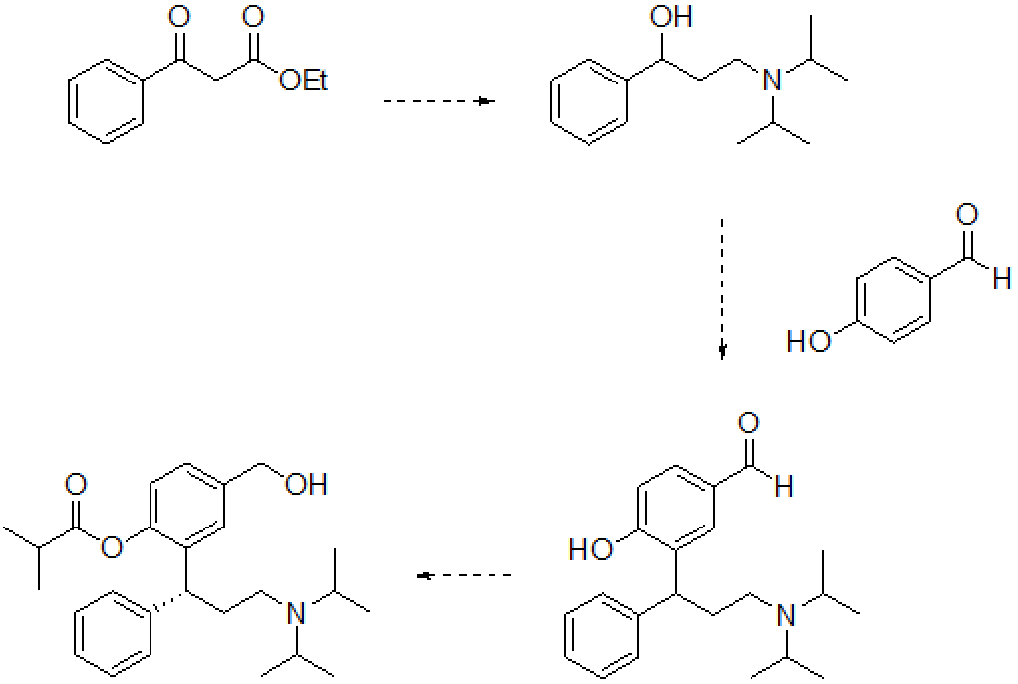
Efficient Synthesis of Fesoterodine

이영은 이학준[1,*]

한양대학교 바이오나노학과 [1]한양대학교 응용화학과

Fesoterodine is a muscarinic receptor antagonist used for the treatment of overactive bladder. It is a congener of tolterodine but it has been shown to appear superior efficacy compared with tolterodine. In this study, we present an efficient synthesis of fesoterodine from ethyl benzoylacetate. After the reduction to 1,3-diol, diisopropylamine substitution, Friedel-Crafts alkylation in presence of acid catalyst as a key reaction step, etc., the synthesis of fesoterodine is completed.



Fesoterodine

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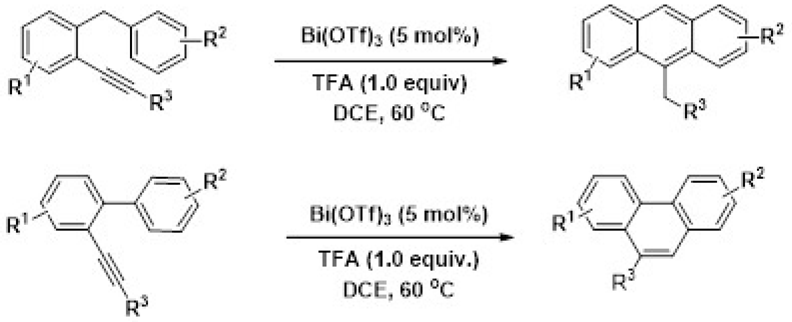
Bismuth-catalyzed synthesis of polycyclic aromatic hydrocarbons

박정민 이구연*

강원대학교 생명건강공학과

Functionalized anthracene and phenantrene derivatives are important structure for potential thrapeutics and polymeric materials. Recently, we developed a concise method for the preparation of anthracenes and phenantrene from o-alkynyldiarylmethane and o-alkynylbiphenyl catalyzed by Bi(OTf)3 in moderate to good yields. Compared to the previous reaction using expensive Au/Ag catalysts, this strategy provides a flexible and efficient route to substituted anthracenes and phenantrenes .



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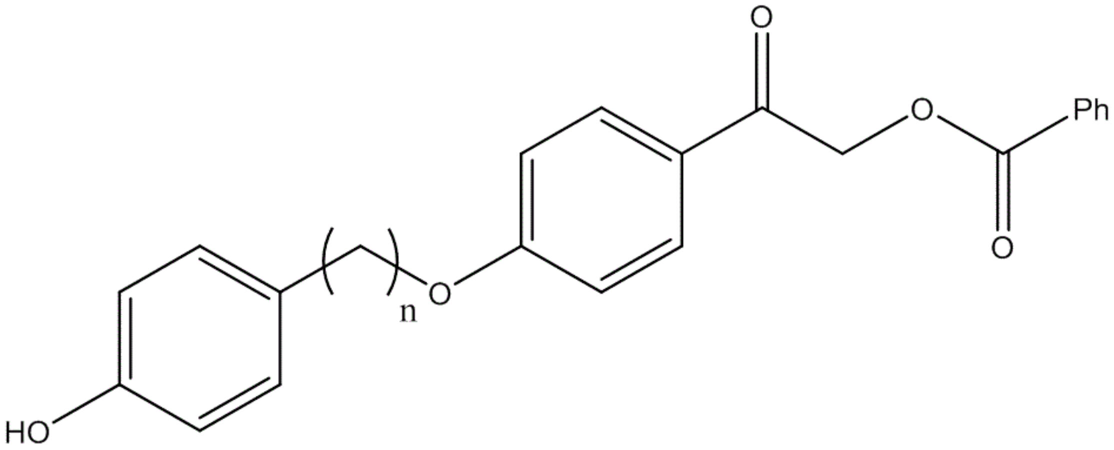
Chain Length Dependence on Photochemistry of 4-Alkoxyphenacyl Benzoates

한관우 오승훈 안세진 조덕희 박봉서*

동국대학교 화학과

Several 4-alkoxyphenacyl benzoates having varied chain length in the para alkoxy group shown below have been prepared and their photochemical properties have been investigated. All the compounds tested release benzoic acid upon photolysis, but the quantum efficiency varies depending upon their chain length. It is suggested that the reaction goes through hydrogen abstraction reaction of triplet excited carbonyl chromophore from remote phenol moiety via a sandwich-like conformation. The mechanistic detail and the origin of the chain length dependence will be discussed using our experimental and theoretical results of this system


O
Ph
O
O
n
HO

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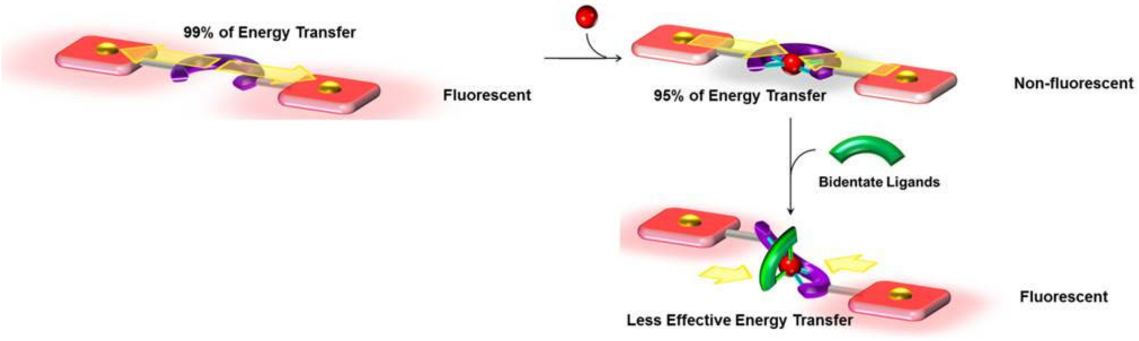
A Porphyrin-based Molecular Tweezer Having Guest-induced Forward and Backward Energy Transfer

윤홍식 임종민 김동호* 장우동*

연세대학교 화학과

A bisindole-bridged-porphyrin tweezer (1) exhibited unique switching in forward and backward photo-induced energy transfer by specific guest bindings. Among various metal ions, the addition of Cu^{2+} only caused a change in electronic absorption and fluorescence quenching of 1. MALDI-TOF-MS and FT-IR analyses indicated the formation of stable coordination complex between 1 and Cu^{2+} (1-Cu(II)). Without Cu^{2+} coordination, the excitation energy flows from biindole bridge (BB) to porphyrin (P_{Zn}), where the energy transfer efficiency was estimated to be 99%. In contrast, the direction of energy flow in 1 was completely reversed by the coordination of Cu^{2+}. The difference in fluorescence quantum yield between 1 and 1-Cu(II) indicates that more than 95% of excitation energy of P_{Zn} flows into Cu(II)-coordinated BB. The energy transfer efficiency was further controlled by bidentate ligand coordination onto 1-Cu(II). When pyrophosphate ion was added to 1-Cu(II), the recovery of fluorescence emission from P_{Zn} was observed. The quantum mechanical calculations indicated that the Cu(II)-coordinated BB has square planar geometry, which can be distorted to form octahedral geometry due to the coordination of bidentate ligands.



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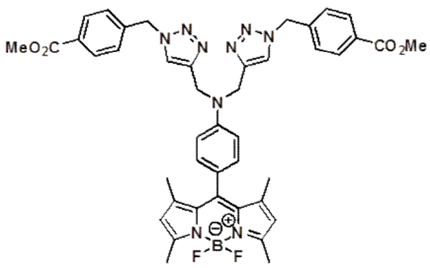
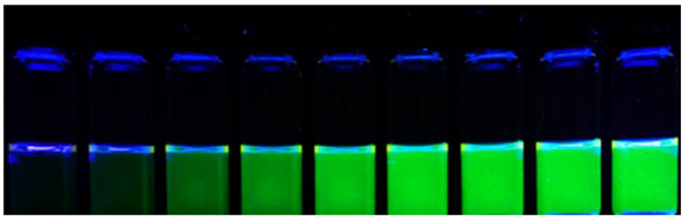
Fluorescent turn-on sensor for the detection of gold species in aqueous media

임다정 윤홍식 장우동*

연세대학교 화학과

Due to the superior processability and many important characteristics, gold currently becomes very important materials in many industrial fields as well as basic science. Although the metallic gold is highly stable, ionic form is very reactive and some organogold compounds exhibit strong toxicity. Therefore, the development of gold chemosensor would be one of the significant topics for the imaging of ionic gold in biological system. Herein, we report a BODIPY-based 'turn-on' fluorescent probe (1) for the detection of gold species, which has the unique photo-induced fluorescence enhancement behavior. We conducted Cu(I)-catalyzed click reaction to get the probe that has two triazole groups. Upon various metal ion additions, Au^+ only caused fluorescence enhancement of 1, indicating high selectivity of 1 to Au^+. On the other hand, the fluorescence intensity of 1 was gradually enhanced by addition of Au^{3+} in $MeCN/H_2O$ (1:1 v/v) under light irradiation. Therefore, we can distinguish not only gold species from other metal ions but also between Au^{3+} and Au^+. We made effort to find out the mechanism and worked on NMR titration under the light of 365 nm, analysis of MALDI-TOF mass spectroscopy and so on.





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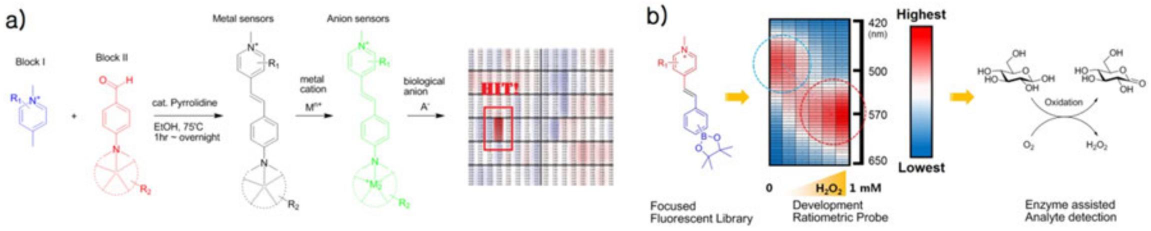
Development of fluorescent probes by focused libraries for metal cations, biological anions, and hydrogen peroxide

이상욱 홍종인*

서울대학교 화학부

Fluorescent probes have been widely used for molecular cellular biology research, disease diagnosis, and environmental pollution detection. The selectivity of a probe is the most important factor in the detection of a specific target among a myriad of analytes. In particular, the detection of a specific biomolecule is challenging because there are a large number of important biomolecules in cells. It is a formidable task to design ultraselective probes that show distinct fluorescent signals for specific analytes because current molecular modeling technology cannot predict both the structure of a probe-analyte complex and the fluorescence signal change upon binding. Recently reported ultraselective probes were developed serendipitously in the course of screening various analytes. First, a focused fluorescent probe library for metal cations was developed by combining metal chelators and picolinium/quinolinium moieties as combinatorial blocks connected through a styryl group. Furthermore, metal complexes derived from metal chelators having high binding affinities for metal cations were used to construct a focused probe library for phosphorylated biomolecules. More than 250 fluorescent probes were screened for identifying an ultraselective probe for dTTP. Second, hydrogen peroxide selective ratiometric fluorescent probes were developed by controlling electron push-pull character of styryl dye-boronate conjugates. One probe from a focused library showed a red-shift of over 100 nm in the maximum fluorescence emission wavelength and an increase in ratio of over 30-fold, upon the addition of H2O2, The probe was successfully utilized for the real-time monitoring of glucose oxidation by glucose oxidase.


a)
Block I
Block II
cat. Pyrrolidine
EtOH, 75℃
1hr ~ overnight
Metal sensors
metal cation
M^{n+}
Anion sensors
biological anion
A^-
HIT!
b)
Focused Fluorescent Library
Development Ratiometric Probe
0
H_2O_2 1 mM
420 (nm)
500
570
650
Highest
Lowest
Oxidation
O_2
H_2O_2
Enzyme assisted Analyte detection

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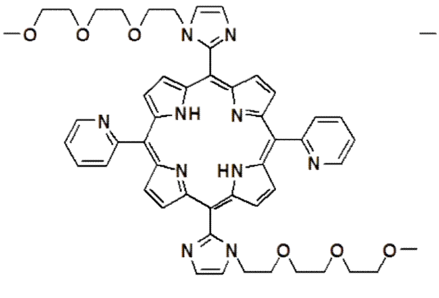
Porphyrin-Based Fluorescence Probe for Detection of Au^{3+} and Cysteine Using Imidazole Moieties

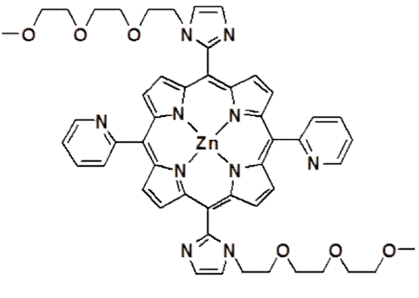
김주호 장우동*

연세대학교 화학과

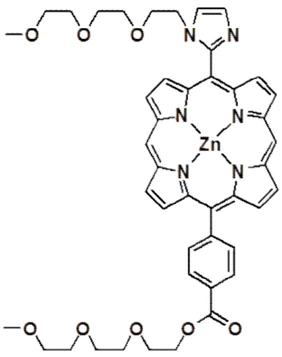
A series of imidazole-bearing porphyrins (P_{FB}, P_{Zn}, Q_{Zn}) were synthesized. Spectral responses of P_{FB} with additions of various metal ions were examined. The additions of Au^{3+}, Hg^{2+}, and Cd^{2+} to P_{FB} caused the spectral changes of UV/Vis absorption. On the other hand, when the same experiments were carried out for P_{Zn}, the addition of Au^{3+} only caused complete florescence quenching. The UV/Vis absorption of P_{Zn} also exhibited clear shift by addition of Au^{3+}.In order to investigate the binding mechanism of Au^{3+} and P_{Zn}, NMR titration study was carried out. However, all ^1H NMR peaks of P_{Zn} were too complicated to assign. To simplify this problem, we newly synthesized a porphyrin having single imidazole moiety (Q_{Zn}). Q_{Zn} gave simple sharp peaks upon the ^1H NMR spectroscopy to verify binding mechanism of Au^{3+} and Q_{Zn}.The quenched florescence of $P_{Zn}\cdot Au^{3+}$ was successively recovered by addition of cysteine, because of the removal of Au^{3+} ion. All other amino acids did not show the recovery of fluorescence emission. Unlike other amino acids, only cysteine has thiol moiety which can bind strongly with Au^{3+}. Finally, we tested in vitro bioimaging of cysteine. P_{Zn} exhibited strong red fluorescence. On the other hand, the fluorescence was hardly detected when the same experiment was carried out using $P_{Zn}\cdot Au^{3+}$. And the cells containing cysteine display strong red fluorescence, indicating $P_{Zn}\cdot Au^{3+}$ successfully works as the fluorescence probe for detection of cysteine in biological evaluation.



P_{FB}



P_{Zn}



Q_{Zn}

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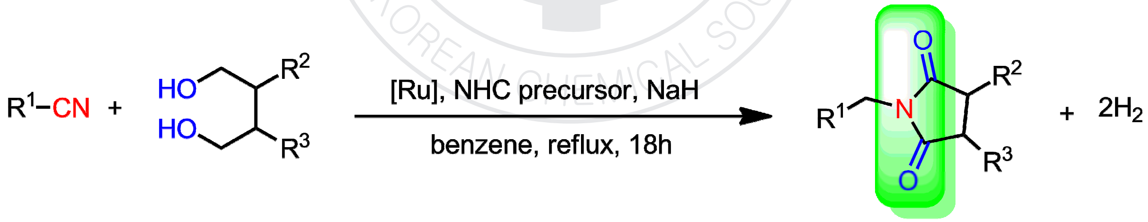
Atom-economical Synthesis of Cyclic Imides from Diols and Nitriles

김재운 홍순혁[1,*]

서울대학교 화학부 [1]서울대학교 화학과

We have developed an atom-economical and versatile protocol for the synthesis of a cyclic imide from a nitrile and a diol, which are readily available and easy to handle. Dehydrogenative alcohol activation by a ruthenium catalyst makes possible direct imide formation between α-carbons of diol and a nitrogen atom of nitrile, liberating two equivalents of hydrogen gas as a sole by-product. This operatively simple protocol will provide a efficient method for the synthesis of various cyclic imides which are attractive candidates for drug development.



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Synthesis of 4-(Benzo[d]thiazol-2-yl)phenyldiphenylphosphine Oxide (4-BDO) as a Blue-Emitting OLED Material

강은국 김경현[1] 이범종[1,*]

인제대학교 화학과 [1]인제대학교 의생명화학과

We have synthesized 4-(benzo[d]thiazol-2-yl)phenyldiphenylphosphine oxide (4-BDO, Fig. 1) as a novel blue-emitting OLED material. The one-pot synthesis of the phosphine-benzothiazole structure was achieved using PPA as solvent and catalyst for the cyclization reaction. The phosphine product was oxidized to 4-BDO with aqueous H_2O_2. The chemical structure of 4-BDO was determined by ^{1}H-NMR, ^{13}C-NMR, FT-IR and UV-vis. The 4-BDO showed a strong blue emission under excitation by UV-lamp of 365 nm. The photoluminescence (PL) and electroluminescence (EL) properties of 4-BDO were investigated.

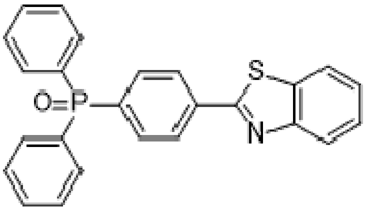

Fig 1. The chemical structure of 4-BDO

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Preparation of highly energetic ionic liquids for chemical propulsion

김중현 조성준[1,*]

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Hydrazine and homologue compounds have been typical and standard propellants in the chemical propulsion for the satellite altitude and attitude control. In the meantime, it is considered as a highly toxic chemical substance with a high vapor pressure. In order to overcome the toxicity problem, new eco-friendly chemical propellant has to be developed. Ionic liquid can be a promising candidate due to the low vapor pressure. Among the various ionic liquids, the dicyanamide anion based diquaternary ammonium ionic liquid shows the superior performance such as ignition delay required for bipropellant application. In this work, several diquat ionic liquids, 1,1'-(ethane-1,2-diyl)bis(1-methylpyrrolidin-1-ium), 1,1'-(propane-1,3-diyl)bis(1-methylpyrrolidin-1-ium) and hexamethylethane-1,2-diaminium were synthesized. The obtained ionic liquids were characterized using ^{13}C and ^{1}H NMR spectroscopy. The chemical and thermodynamic properties was estimated using both semi-empirical and ab-initio calculations, respectively.

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Tandem Synthesis of Amides and Secondary Amines from Esters with Primary Amines under Solvent-Free Conditions

이정빈 홍순혁[1,*]

서울대학교 화학부 [1]서울대학교 화학과

Iridium(III)-catalyzed tandem synthesis of amides and amines from esters under solvent-free conditions is described. Commercially available [Cp*IrCl2]2 with NaOAc showed the best activity for the synthesis of amides and secondary amines. Amide was formed by ester-amide exchange which generates alcohol in situ thereby secondary amine was formed via hydrogen autotransfer. This synthetic protocol with high atom economy generates water as the sole by-product and can afford amides and amines from various esters in one-pot reaction, expanding the synthetic versatility of ester transformations.

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TFA-assisted Deletion of N-acylated Peptoids

김수민 권용억*

이화여자대학교 화학.나노과학과

Peptoids are the structural isomers of peptides with the alkyl substitution at the amide nitrogen instead of ?-carbon of peptides. Peptoids are endowed with diverse structural and functional features and in many cases, peptoids are even more advantageous to the corresponding peptides due to easy chemical synthesis, improved cell permeability, proteolytic resistance, and tolerance towards high salt concentration, organic solvents, and extreme pH. Thus, peptoids have emerged as an attractive class of peptidomimetics in chemical biology, molecular biophysics, drug development, and medical diagnostics.When peptoids have been used as chemical tools in biological application studies, the terminal amino group has often been protected with acetyl groups. The protection of the N-terminal group makes peptoids more hydrophobic, which is known to improve cell permeability, therapeutic potential, etc. In addition, in the case of the solid-phase RCM which we recently reported, the terminal amino functional group of peptoids should be protected with acetyl or Boc groups prior to the RCM step to prevent the poisoning of the Ru catalyst. Interestingly, the unusual deletion of the terminal peptoid unit has sometimes been encountered when the acetylated linear peptoids were treated with a trifluoroacetic acid (TFA) cleavage cocktail. Therefore, we report herein systematic studies on the scission of N-acylated peptoids, which could rationalize the formation of the deleted peptoids and also establish an appropriate strategy to minimize such undesired deletion.

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Synthesis of New Clover-type Dendrimers via Dual Click Chemistry

윤성희 한승철 이재욱*

동아대학교 화학과

Click chemistry, which is the Cu(I)-catalyzed Huisgen [2+3] dipolar cycloaddition reaction between an organic azide and a terminal alkyne, has found many applications in combinatorial and organic chemistries, material science, and synthesis of polymer and dendrimer. The reaction, characterized by very high yields, mild and simple reaction conditions, excellent oxygen and water tolerance, and simple product isolations, is highly chemoselective affording only the desired 1,2,3-triazole even in the presence of a large variety of other functional groups. Therefore, the click chemistry as a concept of simplifying synthesis is very useful tool to produce functional polymers and dendrimers. In addition, Staudinger/aza-Wittig reactions (new click reaction) are a powerful tool in organic synthetic strategies directed towards the construction of nitrogen-containing compounds. Recent investigation of the click chemistry, the Staudinger/aza-Wittig reaction between an organic azide and an aldehyde, has attracted attention which has found many applications in organic chemistry, materials science and synthesis of various dendrimers. Taking advantage of these facts, herein we report result in synthesis of new clover-type dendrimers containing four dendrons of the different generations via dual click chemistry with the copper-catalyzed cycloaddition and Staudinger/aza-Wittig reactions.

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Ratiometric probe for the determination of a wide range of pH values in cells

박나영 이재홍 권보미 엄수진 강철훈[1,*] 김종승[*]

고려대학교 화학과 [1]경희대학교 동서의학대학원

A chameleon fluorescent pH probe composed of both fluorescein and rhodamine units was synthesized in high yield and used to visualize organelles in cells having different pH values. We observed that the cyclolactam rings of rhodamine and fluorescein open in acidic and in neutral-basic media to give fluorescence emission at 580 and 512 nm, respectively. We also found that a plot of the ratio F_{512}/F_{580} versus acidity in the pH range 4-8 was linear, which covers most physiological pH values. Confocal microscopic images of HeLa cells labeled with the probe revealed two distinct emission ranges at 500-550 nm (green) and at 555-650 nm (red), corresponding to neutral-basic and acidic organelles within the cell, respectively. Colocalization experiments confirmed that the red fluorescence of the probe overlapped with a lysosomal dye and the green fluorescence corresponded to basic organelles in the cytoplasm. From the pH-dependent calibration curve of the fluorescence changes of the probe, the lysosomal pH value of HeLa cells was estimated to be 5.7±0.2, which could be changed by adding H_2O_2 or NAC. This lead us to conclude that the pH value of the lysosomes could be controlled by the cellular redox balance. Therefore, the probe gives a dramatic change in the relative fluorescence intensity of its two fluorophores over a wide pH range and could be an ideal diagnostic method for measuring pH fluctuations in pathogenic cells.

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Organocatalytic Asymmetric Synthesis of Chiral Pyrrolizine-Based Triheterocycles by A Cascade Reaction

이효준 조창우*

경북대학교 화학과

Methods for the construction of polyheterocyclic skeletons have been the focus of intensive research efforts because of their diverse structural features and interesting biological activities. In particular, the development of efficient routes for the asymmetric synthesis of stereogenic complex molecules including chiral polyheterocycles from simple starting materials in a single step has become a challenging topic in modern organic chemistry. In this regard, we recently reported organocatalytic asymmetric cascade aza-Michael-aldol reactions of α,β-unsaturated carbonyl compounds with pyrroles as *N*-centered heteroaromatic nucleophiles to provide a variety of chiral pyrrolizines. Owing to the importance of pyrrolizines in the development of pharmaceuticals, we planned to prepare chiral pyrrolizine-based polyheterocycles as a unique and potential skeleton of pharmaceutical agents. Herein, we report the organocatalytic asymmetric cascade aza-Michael-aldol reactions of α-branched α,β-unsaturated aldehydes with trifluoroacetylpyrroles as *N*-centered heteroaromatic nucleophiles that afford highly functionalized chiral pyrrolizine-based triheterocycles having two quaternary stereocenters of three consecutive stereocenters. Concomitantly, two sequential Suzuki cross-couplings of the chiral pyrrolizine-based triheterocycles with different aryl boronic acids provide unsymmetrically diarylsubstituted chiral pyrrolizine-based triheterocycles in a highly chemoselective controlled manner.

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Asymmetric Organocatalytic Aza-Michael Reactions of Pyrazoles with Enones

이수정 조창우*

경북대학교 화학과

Pyrazole is important skeleton that exhibit a variety of interesting biological activities and thus have found application in the development of pharmaceuticals such as Celebrex and Zoniporide. However, the use of pyrazole as the *N*-centered heteroaromatic nucleophile remains almost unexplored in organocatalytic asymmetric reactions, in spite of the importance of pyrazole as optically pure *N*-heteroaromatic pharmacophores in biologically active natural products. Here, the use of pyrazoles as the *N*-centered heteroaromatic nucleophiles in the organocatalytic asymmetric aza-Michael reactions of enones will be presented.

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Asymmetric Organocatalytic Synthesis of Chiral 2-Isoxazolines by A Cascade Reaction

윤희석 조창우*

경북대학교 화학과

2-Isoxazolines are an important class of heterocyclic compounds that show a variety of remarkable biological activities and thus have found application in the development of pharmaceuticals. Recently, the development of organocatalytic asymmetric cascade reactions has received much attention, because they provide powerful tools for the concise construction of complex structures from simple precursors in a single step. Herein, we report the asymmetric synthesis of 2-isoxazolines by the organocatalytic cascade oxa-Michael/imine cyclization reactions of (*E*)-tert-butyl 2-methyl-4-oxo-4-(hetero)arylbut-2-enoate as the substrates with hydroxylamine as the nucleophile.

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Chiral Primary Amine-catalyzed asymmetric Aza-Michael Reactions of Enals with Pyrroles

안준기 조창우*

경북대학교 화학과

Pyrroles are an important class of heterocycles that display a variety of remarkable biological activities and thus have found application in the development of pharmaceuticals. In organocatalytic asymmetric reactions, the use of pyrroles as *N*-centered heteroaromatic nucleophiles remained unexplored in contrast to the widely studied *C*-centered nucleophiles. However, recently, we reported the chiral prolinol trimethylsilyl ether-catalyzed asymmetric aza-Michael reactions of pyrroles as the *N*-centered heteroaromatic nucleophiles to α,β-unsaturated aldehydes. As the expansion of the organocatalytic asymmetric aza-Michael reactions with pyrroles as the *N*-centered heteroaromatic nucleophiles, we report the cinchona-based primary amine-catalyzed asymmetric aza-Michael reactions of pyrroles to α,β-unsaturated aldehydes.

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Cyclization of Isobenzofuran-1-(3H)-ones with o-Phenylenediamine or Heteroaromatic diamines

Cyclization of Isobenzofuran-1-(3H)-ones with o-Phenylenediamine or Heteroaromatic diamines

권연근* 이도훈 정대일 한정태[1]

동아대학교 화학과 [1]영동대학교 뷰티케어과

1,4-and 1,5-benzodiazepine scaffolds structures have already proven their utility in medicinal chemistry. Recent trends in drug discovery show an attempt to move away from flattened aromatic structures to their saturated counterparts. Implementation of this idea to 1,4 and 1,5-benzodiazepine scaffolds, as well as to their fused analogues gives rise to three-dimentional molecular frameworks which potentially might preserve the 'privileged' status of their aromatic preunsorp. Herein, we report two-step reaction sequence for the preparation of isoindolo[2,1-a][1,5]benzodiazepin-1,2-ones. pthalaldehydic acid has been prepared by the alkaline oxidation of naphthalene. Cyclization of isobenzofuran-1-(3H)-ones with o-phenylenediamine or heteroaromatic diamines led to the formation of isoidolo[2,1-a][1,5]benzodiazepin-1,2-ones.

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Carbazole-Based Turn-off Fluorescent Chemosensor for Heavy Metal Ion Detection

황인환 장우동*

연세대학교 화학과

There are many causes of environmental pollution. Among various pollutants, heavy metal ions are of great concern because they generally tend to accumulate in living organisms. Even if low concentrations, they cannot be degraded and represent a serious health problems. Therefore, the development of selective and sensitive methods for the determination of heavy metal ions is currently receiving considerable attention. Heavy-metal ions (e.g., Hg^{2+}, $Ni2^{2+}$,Cd^{2+}, Pb^{2+}, Cr^{2+}, Cu^{2+}, etc.) are one of the most toxic and carcinogenic pollutants. Existing several detecting methods reveal the limitation to expensive equipment and to involve time-consuming and laborious procedures by trained professionals As a result, there is an urgent need for low-cost, highly sensitive and selective methods of discrimination of heavy-metal ions. In this study eight carbazole-based compounds were synthesized as chemoselective chromophores for metal bindings. The carbazole-based compounds exhibited different patterns of fluorescence emissions against the additions of 14 heavy metal ions.

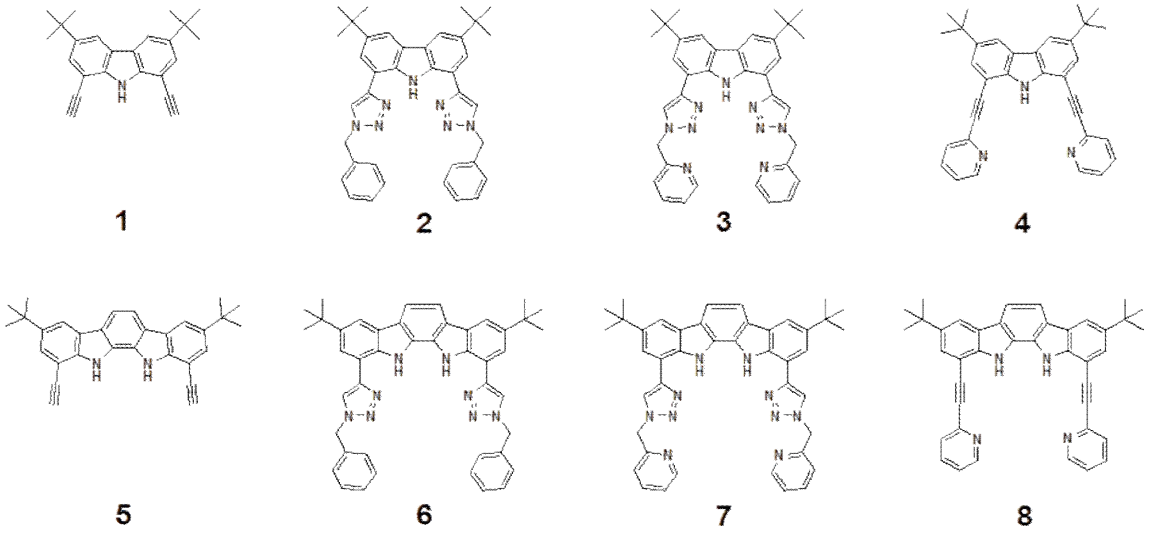

Figure 1. Carbazole-based chemoselective chromophores

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Nano/microstructures generated by self-assembly of photoisomerizable azobenzenes

Mina Han[*] **Takahiro Seki**

Nagoya University

The design and creation of photoswitchable nano/microstructures have received much attention in the fields of photochemistry, nanotechnology, biology, organic chemistry, and so on. Among the various types of photochromic molecules, considerable interest has been focused on azobenzene due to its structural change between the trans and cis forms and its ease of chemical modification. The trans form stabilizes crystalline and liquid crystalline (LC) phases, whereas the cis form destabilizes the crystalline and LC phases. Accordingly, irradiation with ultraviolet (UV) light may cause an isothermal LC-to-isotropic phase transition in an aggregated state. Nevertheless, there are only a few reports on solid azobenzene compounds which liquefy under UV light at room temperature. Recently, we have designed a crystalline azobenzene monomer which becomes liquid at ambient temperature by UV light irradiation. We confirmed that the synthetic sphere assembled from the azobenzene monomer undergoes light-directed morphological transformation between spherical and disassembled states. The light-responsive sphere system can be applied to drug delivery and emerging separation systems which require on-demand encapsulation/release at a specific light wavelength.In addition, to gain an understanding of fluorescent azobenzene-based aggregates, we have synthesized distorted azobenzene derivatives, in which sterically hindered phenyl rings are connected to a central aromatic core through the azo groups. The compounds assemble into one dimensional (1D) fibers. The formation of 1D fiber does not weaken the fluorescence intensity, but rather the intensity is increased by ~4 times. Moreover, the fluorescence from the fibers can be readily switched off by pressing or scratching.

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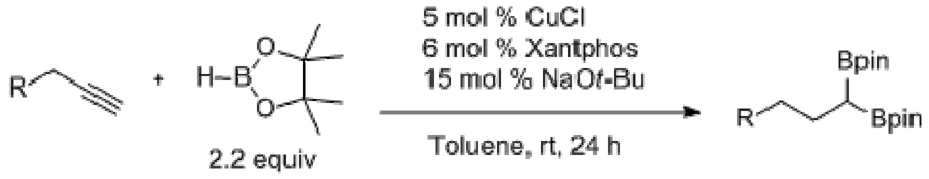
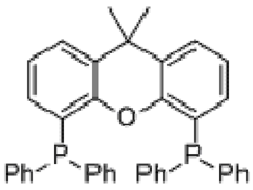
Highly Regioselective Synthesis of *gem*-Organodiboronates by Copper(Ⅰ)-Catalyzed Hydroboration of Terminal Alkynes

이수민 **LI DINGXI** 윤재숙[*]

성균관대학교 화학과

Boronate compounds can be easily converted into alcohols, amines, and carboxylic acids, and also used for the formation of C-C bond. *Gem*-organodiboronates have unique reactivity and would be fascinating synthetic intermediates for the further functionalization. Recently, Shibata and co-workers reported Rh(Ⅰ)-catalyzed sequential regioselective hydroboration of 1-alkynes. But their reaction produced not only 1,1-organodiboronates but also reduction products as a side product.We tried to develop highly regioselective synthesis of *gem*-organodiboronates by copper catalyzed sequential hydroboration of various terminal alkynes. The target molecules were prepared in one step without the formation of undesired regioisomer and reduction product.





Xantphos

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A Study on the Synthesis of 2-Amino-4-arylthiazoles and 2-Substituted-4-arylthiazoles

김수완 정대일* 한정태[1] 송주현

동아대학교 화학과 [1]영동대학교 뷰티케어과

It's well known that thiazole devatives are important compounds in medicinal chemistry due to their broad range of biological activities. Thiazoles are found in a variety of specialized products, often fused with benzene derivatives, the so-called benzothiazoles. This type of heterocycles have shown wide variety of pharmaco active protecties as anti-inflammatory, anti-tubercular, antibacterial, fungicidal, local anesthetic, tranquilizers, insecticidal, anti-microbial, anti-tumor and diuretic. Considerable efforts have been devoted to the synthesis of this type of compounds. Taking in consideration the advantages of microwave heating on solvent-free reactions, we report the rapid solventless synthesis of a series of 2-amino-4-aryl-1,3-thiazoles under microwave irradiation, prepared from the cyclocondensation of heteroaromatic ketones with thiourea and iodine. And also we report the reation of synthesized 2-amino-4-arylthiazole with 2,5-dimethoxytetrahydrofuran and 1,3-acetonedicarboxylic acid.

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A study on the Synthesis of 2-Substituted 4-phenyl quinolines And 3,9-dihalogen-6,12-bis(3-halogenphenyl)dibenzo[b,f][1,5]diazocine

김성태 김인식[1] 이용균 정대일[*] 한정태[2]

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Quinolines are well known not only for their significant biological activities but also for their formation of conjugated molecules and polymers that combine enhanced electronic, optoelectronic, or nonlinear optical properties with excellent mechanical properties. Quinolin used to manufacture preventing pellagra diseases of human nicotinic acid and other compounds.Recently, much attention has focused on microwave assisted organic reaction in the absence of solvent. Often, thermal demanding reactions take hours in solution, and may require repetitive treatments with excess reagents to drive them to completed in minutes. We report synthesis of 2-substituted 4-phenylquinoline derivatives by using dihalogen substituted 2- aminobenzophenones and aromatics having acetyl group for 5 minutes under microwave irradiation.

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Copper catalyzed γ-Oxyamination of aldehydes via Dienamine intermediate

정원지 장혜영[1,*]

아주대학교 에너지시스템학부 [1]아주대학교 화학과

Organocatalysis of asymmetric C-O bond formation with various aldehydes and free radical 2,2,6,6-tetramethylpiperidine N-oxyl (TEMPO) was carried out with a combination of copper catalyst and acid additives to afford γ-oxyminated aldehyde in good yields. Furthermore, an efficient tandem reaction system was developed, in which primary alcohols underwent oxidation to give the corresponding aldehyde and subsequent γ-oxyamination occurred.

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N-Heterocyclic Carbene Catalysed Oxidative Esterification and Thioesterification

지미란 장혜영[1,*]

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The utility of the TEMPO oxidant was expanded to various oxidative processes under metal-free carbene-catalysed conditions. Utilization of N-heterocyclic carbene and 2,2,6,6,-tetramethylpiperidine N-oxyl (TEMPO) is proposed for the synthesis of esters and thioesters. Even though TEMPO was used as a stoichiometric oxidant, various exogenous alcohols and benzyl mercaptan were allowed to react with aldehydes to afford esters and thioesters. In particular, our oxidative catalytic system promoted unexpected dehydrogenation of saturated aldehydes to give α,β-unsaturated esters.

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Side Chain Functionalization of Peptoids via Suzuki-Miyaura Cross-Coupling Reaction

남호연 서지원[1,*]

광주과학기술원(GIST) 화학과 [1]광주과학기술원(GIST) 기초교육학부

Peptoids constitute a class of peptide biomimetic molecules based on oligo-N-substituted glycines. As a bioinspired material, peptoids have shown wide applications including biologically active molecules, catalysts, sensors, and artificial proteins. The main research of peptoids is to utilize them as a scaffold to display various functional groups emphasizing the importance of novel conjugation methods. Herein, we demonstrated that peptoids could be readily decorated at side chains with diverse functional groups employing Suzuki-Miyaura cross-coupling reaction (or Suzuki coupling). Suzuki coupling provides a direct carbon-carbon bond between peptoid side chain and a functional group, and orthogonal conjugation reaction conditions which enable selective side chain functionalization. Peptoid side chain decoration was performed on a solid phase resin using $Pd(PPh_3)_4$ and K_2CO_3 in NMP solvent, at 80 ºC for 1 hour, showing the best conversion of 73 %. The usefulness of this method was demonstrated by a multivalent display of pyrenes on a peptoid helix, which exhibited a permanent excimer formation.

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Self-Assembly and Spectroscopic Analysis of Porphyrin-Peptoid Conjuagtes

강보영 서지원[1,*]

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Peptoids are a class of peptidomimetic polymers based on oligo-N-substituted glycine backbones. As a bioinspired heteropolymer, peptoids have advantages in precise control of chain length, side chain functionality and monomer sequence. Porphyrin?peptoid conjugates (PPCs) are porphyrin displayed molecules using peptoid as a scaffold. Distance, orientation, and number controlled porphyrin-peptoid conjugates (PPCs) were efficiently synthesized. Each PPC showed distinct degree of J-aggregation in visible absorption spectra profiles depending on the mode of display of porphyrins. Another evidence of porphyrin interactions was appeared in circular dichroism signature as negative Cotton effects at the Soret region. Further spectroscopic studies were performed focusing on self-assembly of PPCs. The concentration and temperature dependency of red-shifted visible spectra of PPCs revealed the existence of aggregate species of PPCs, in other words, self-assembly of PPCs. Thermodynamic interpretation was attempted to analyze aggregation process of PPCs. Concentration dependent fluorescence emission also showed evidences of self-assembly of PPCs. Quantum yield and extinction coefficient at 414 nm of each PPC were measured.

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Sovatochromic Study of Spiropyran-Cored PAMAM Dendron and Colorimetric Sensing for Cu(II) Cation

신은주* 허대영

순천대학교 화학과

Solvatochromism refers to the solvent-dependent change in position of the absorption bands, caused through the modification of the energy gap between the ground states and excited states by the solute-solvent interactions. Merocyanine has been known to display negative solvatochromism, meaning a blue shift of absorption bands in solvents of increasing polarity. The solvatochromism of merocyanine has been studied for its potential use as an empirical indicator of solvent polarity. Despite the potential applications of spiropyrans, most studies focused on utilizing monomeric, simple spiropyrans. Some functionalized spiropyrans will be more useful in practical applications. Copper is one of the three most abundant and physiologically essential transition metal ions in the human body. However, excessive amounts of copper can cause serious health problems such as kidney failure, nerve system damage, or even death. Therefore, developing better sensors for the detection of environmentally and biologically copper has been an important subject in the field of chemical sensors for several decades. Incorporating photochromic molecules into PAMAM dendron might lead to a light-modulated sensor. Spiropyran-cored PAMAM dendron shows solvatochromic behavior in various solvents, reversible photochromic reaction, and acts as a copper(II) ion-selective sensor.

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Cyanide-Selective Sensor Based on Porphyrin-Spiropyran Dyad

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순천대학교 화학과

Incorporating a photochromic molecule SP into porphyrin could lead to interesting photoresponsive system, the properties of which can be manipulated by both light and solvent. Por-SP dyad conducts solvent-dependent photoreactions, ring-opening reaction in THF (Por-SP to Por-MC, red to violet) and protonation in dichloromethane(Por-SP to H2Por2+-SP, red to green). Anions play important roles in the areas of biological and environmental chemistry. The design of selective sensors to detect the targeted anions has attracted a great attention. In particular, there is a strong need for the development of sensors for cyanide detection, because the cyanide anion is one of the most hazardous contaminants and extremely toxic to living organisms.In this study, CN- selective sensing ability based on Por-SP dyad was investigated using absorption and fluorescence spectroscopy.

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Preparation, Photochromic Reaction, and Ion Sensing of Rhodamine-Spiropyran Dyad

신은주* 허대영

순천대학교 화학과

Rhodamine(Rh) derivatives are excellent fluorophores and chromophores. They have attracted considerable interest due to their long absorption and emission wavelengths elongated to the visible region, high fluorescence quantum yield, and large absorption coefficient. Generally, in presence of specific metal ions, the colorless and nonfluorescent rhodamine spirolactam structure would be converted into the colored and highly fluorescent ring-opened amide form, which provides not only excellent enhancement in absorption and fluorescence intensity, but also direct visual detection. Nonpolar, colorless, spiropyran(SP) is well-known photochromic compound accomplishing reversible molecular structural change to polar, colored, merocyanine(MC) by the photochemical heterolytic C-O bond cleavage on UV irradiation. In turn, MC is reversed to SP by rebinding upon thermally or irradiation of visible light. Moreover, spiropyrans have been known to detect selctively some metal cations and anions. Reversible photochromic SP-MC transformation is one of subjects of active research on non-linear optics, data recording, electical and optical switching, and chemical sensing, among others. Incorporating SP into Rh might should lead to excellent light-controlled ion sensing system. In this study, Rh-SP dyad was prepared and their ion sensing ability was investigated using absorption and fluorescence spectroscopy.

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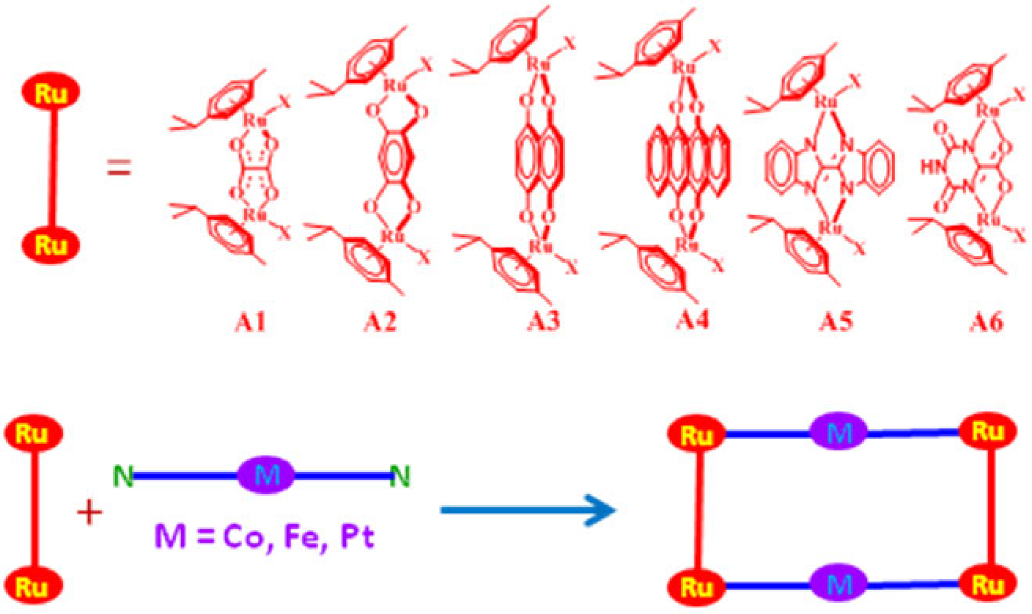
Heterometallic Self-Assembled Metallacycles based on 4-Pyridyl Donors and Arene-Ruthenium(II) Acceptors

SINGH NEM 조재호 지기환*

울산대학교 화학과

In the past two decades, coordination-driven self-assembly has emerged as an effective tool for constructing functionalized metalla-supramolecules with promising applications in molecular recognition, separation, catalysis, encapsulation of guests and biological systems. The present work demonstrates the spontaneous formation of metal?ligand bonds in solution, transforming molecular building blocks into 2D metallacycles using cobalt sandwich compound, ferrocene and platinum derived 4-pyridyl donors and different arene?ruthenium acceptors (scheme 1). The resulting supramolecular complexes have well-defined internal cavities to stack planner aromatic guests. These self-assembled metallacycles were also evaluated for biological activities. All the new complexes have been characterized by various spectroscopic and X-ray single crystal structure determination. The poster will address a detail comprehensive account of the mentioned work.



Scheme 1: Synthetic route to the self-assembled metalla-rectangles

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Preparation and Photochromic Reaction of Spiropyran-Fluorescein Dyad

신은주* 김빛나

순천대학교 화학과

Aluminium is frequently used for an kitchen utensil, foil, stoneware. Also, it is useful as an anti-acid and anti-inflammatory analgesic drug when we have a sour stomach. However, the accumulation of excessive amounts of aluminium in body could result in neurodegenerative diseases for humans, such as Alzheimer's disease, morbid sensitiveness, memory lapse, and forgetfulness. Moreover, it can cause serious health problems such as calcium metabolism disorder, decreased renal function, or even death. Therefore, the development of aluminum sensor is important.Spiropyran(SP) are one of the most widely studied classes of photoswitchable compounds, undergoing reversible structural transformation between a colourless SP form and a coloured merocyanine (MC) form upon light, heat or chemical stimulus, which has been shown to exhibit extremely sensitive absorption and colour changes in the visible range.Fluorescein(Fl) is highly fluorescent and widely used as a fluorescent tracer for many applications and a useful fluorescence probe for important biomolecules, and also known as a color additive. Incorporating Fl into SP is expected to lead to excellent light-controlled fluorometric ion sensing system. In this study, SP-Fl dyad, a spiropyran derivative with fluorescein unit, was prepared. Their spectroscopic properties, photochromic reaction, and ion sensing were investigated using absorption and fluorescence spectroscopy.

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Identification of Immobilizing Glucose Oxidase onto Silica Surface with High Efficiency by Chemical Modification method

오명은 심용균 전철호*

연세대학교 화학과

Recently we developed chemical modification method(CM method) to immobilize Glucose Oxidase onto silica surface, which consists of two steps: coupling of GOx with methallylsilane coupling reagent and catalytic immobilizing modified GOx onto silica surface. In this method, the use of large amount of NHS-ester-functionalized methallylsilane causes the decrement activity of enzyme. We thought activity diminution occurs since excess unreacted silane reagent blocks immobilization site of silica surface. This can be proved by reacting fluorescing dansyl derivative with unreacted coupling reagent that is immobilized onto silica and measuring its fluorescence intensity. To remove unreacted NHS-ester-functionalized methallylsilane for greater loading rate, amino group immobilized silica (scavenger) is used. As a result, we obtained immobilized GOx onto silica surface with high efficiency.

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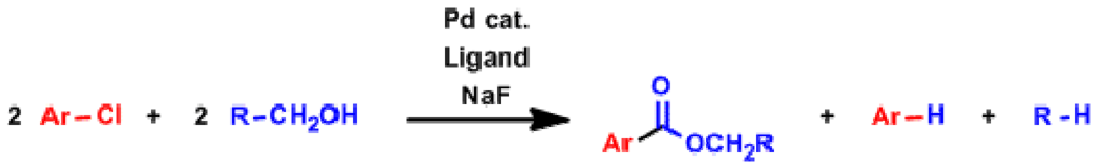
Decarbonylative Esterification from Aryl Chlorides and Aryl Alcohols with Palladium Catalysts

박효순 김동수 전철호*

연세대학교 화학과

Palladium-catalyzed esterification of aryl chlorides through carbonylation has a difficulty because carbon monoxide makes Pd(0) electron deficient. Thus, harsh reaction conditions such as carbon monoxide with high pressure and unusual ligands are required. Consequently, these reactions have practical constraints due to toxicity of carbon monoxide and cost of unusual ligands. In order to enhance these disadvantages, a new type of esterification was developed. In this report, we will describe a new synthetic strategy for esterification from aryl chlorides and aliphatic alcohols. Interestingly, aryl chloride plays a dual role in this reaction; alcohol oxidation with aryl chloride(oxidant) and a substrate. Proposed reaction mechanism will be discussed.



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A New Synthetic Strategy for Carboxylic Ester via Ruthenium-Catalyzed Hydroesterification using Sodium Formate, Olefin and Alcohols

박우진 이창희 김동수 전철호*

연세대학교 화학과

Transition metal catalyzed C-H bond activation has been frequently used as a key method in the development of selective C-C bond formation. Especially, hydroesterification reaction is an important process in synthetic organic chemistry. However, the most of hydroesterification requires toxic carbon monoxide gas with high pressure. To conquer this limitation, we used sodium formate as a carbonyl source substituent of carbon monoxide gas because formates are less toxic and can be handled much more easily than carbon monoxide gas. Recently hydroesterification reactions by using 2-pyridylmethyl formate as a chelating substrate or benzyl formate were reported. In these methods, harmful by-product such as phenol could be produced. In this report, we devise new strategy for hydroesterification using sodium formate, olefin and alcohol in the presence of triruthenium dodecacarbonyl and 2-pyridinemethanol produces carbocylic ester derivatives.

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Doubly Cyclometallation of Ru(II), Rh(III) and Ir(III) Organometallic Complexes and Their Supramolecular Self-assemblies

PALANIELUMALAI 송영호 지기환*

울산대학교 화학과

The design and synthesis of cyclometallated metallacycles of platinum group metals (Pt, Ru, Rh, Ir, and Os) got high attention due to their potential in photofunctional materials such as photocatalysts, dye-sensitized solar cells, electroluminescent devices, and sensors.[1] In particular; the *organometallic* based metallacycles are promising candidates for the above mentioned applications. However, the biological applications such as cytotoxicity, cellular uptakes, bioimaging studies and anti-tumor properties of the cylometallated organometallic complexes are scare.[2] It is well documented that photophysical properties of metal based supramoleculra self-assemblies can be altered by tuning the properties of coordinated ligands. As a continuation of the research on metal based supramolecular self-assemblies of N-donor ligands we introduce new flexible di-topic benzimidazolyl core containing ligands, very recently found that introducing benzimidazolyle units in flexible ligand alter the photophysical and antitumor properties of the metallacycles.[3] Herein, a new family of metallacycles functionalized with benzimidazole units at the cyclometallation ligand is reported. The ligands and cyclometallated organometallic complexes were characterized by analytical and spectroscopic methods will be presented.

References:
[1] Han, Y-F.; Jin, G-X. Chem. Soc. Rev. 2014, DOI: 10.1039/c3cs60343a
[2] Cook, T. R.; Vajayee, V.; Lee, M. H.; Stang, P. J.; Chi, K-W. Acc. Chem. Res. 2013, 46, 2464.
[3] Rajakannu, P.; Elumalai, P.; Shankar, B.; Hussain, F.; Sathiyendiran, M.; Dalton Trans. 2013, 42, 11359.

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A Solvent Effect on the Structure of Coordination-Driven Self-Assembly

이혜우 김동환 지기환*

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Coordination-driven self-assembly is an efficient method for the generation of peculiar supramolecular self-assemblies in a range of shapes and sizes. Various triangles, rectangles and other 2D or 3D supramolecules have been synthesized by this methodology during the last several decades. Supramolecular self-assembly is a spontaneous binding process in various solvents by using one or more non-covalent weak interactions such as H-bonding, π-π interaction, van der Waals force and metal?ligand coordination. Herein, we want to discuss solvent effect as a key factor in controlling the structure of self-assembled metalla-rectangles. In addition, synthesis and characterization of new metalla-rectangles, M_2L_2- and $(M_2L_2)_2$- type, self-assembled with a 9,10-bis[2-(4-pyridyl)ethynyl]anthracene N-donor and arene-Ru acceptors will be also presented in this poster.

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The Synthesis of Benzimidazoles from Benzylamine and Heteroaromatic diamines

김건우 이언진[1] 최순규[1] 정대일[1,*] 한정태[2]

동아대학교 화학 [1]동아대학교 화학과 [2]영동대학교 뷰티케어과

Benzimidazole moiety plays an important role in chemistry and is also present in a variety of biologically active and therapeutically useful compounds. A simple and efficient transformation using readily available reagents under solvent-free and metal-free conditions is considered as a key solution for pollution problems generated by large-scale reaction. In contract to oxygen, which in a biradical in the ground state, sulfur in less reactive. Consequently, the reaction using sulfur present a low risk of explosion, show different and interesting reactivities and selectivities even without metal catalyst, and do not require pressurized reactors. Here in, we report a chemoselective method for an oxidative coupling reaction of alkylamine with various heteroaromatic diamines for the formation of benzimidazole.

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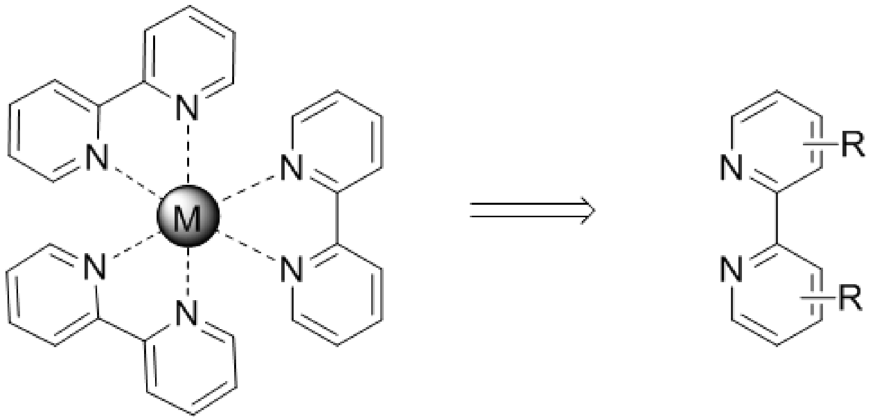
The convenient preparation of Bipyridine Ligand Derivatives: Application for Redox Flow Battery

김기우 안철진* 김은선

창원대학교 화학과

The iron redox flow battery is a type of rechargeable flow battery that employs iron ions in different oxidation states to store chemical potential energy. To improve the energy density, we try to prepare iron complex including bipyridine ligand. In this paper, we will present the efficient preparation of various bipyridine derivatives.



R=COOH, CO_2Et, Br, NO_2, OMe, NH_2

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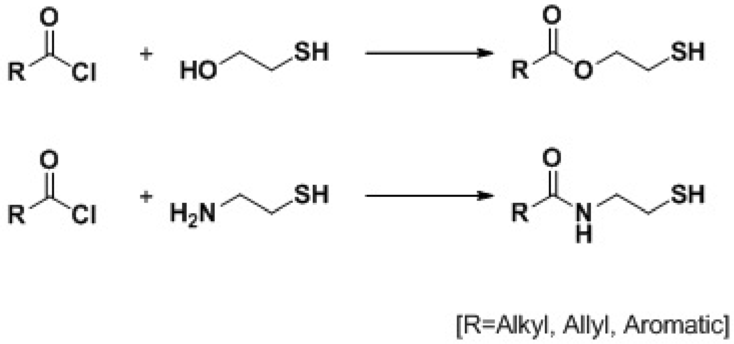
The Investigation and mechanistic study of Chemoselective O-Acylation of β-mercaptoalcohol and N-Acylation of β-mercaptoamine with Acid Chloride Derivatives

김예진 안철진*

창원대학교 화학과

Molecules including free -SH are important to prepare gold nanoparticle(GNP) encapsulating with organic ligand. The selective O-acylation of mercaptoalcohol and N-acylation of β-mercaptoamine are synthetically important to prepare the organic compounds with free -SH. In this paper, the investigation to the chemoselective O-acylation of β-mercaptoalcohol and N-acylation of β-mercaptoamine with acid chloride derivatives and mechanistic study are reported.



[R=Alkyl, Allyl, Aromatic]

일시: 2014년 4월 16~18일(수~금) 3일간
장소: 일산KINTEX
발표코드: **ORGN.P-699**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis of Contrast Agent nanoparticles with Dual T1 and T2 effects for MRI

김범태* 김준영[1] 정유진[1]

전북대학교 생리활성물질연구소, 생리활성소재과학과 [1]전북대학교 생리활성소재과학과

The synthesis of contrast agent with dual T1 and T2 effects was performed. Thus, monocrystalline iron oxide nanoparticles (MION) with T2 effect were coated with dextran and subsequently surfice-modificated with epichlorohydrin, which were finally conjugated with DOTA-Ga3+ complex with T1 effect via Click reaction. Two modular structures were coupled through a proper length of linker, i.e. polyethyleneglycol(n=6)-ethylenediamine.

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장소: 일산KINTEX
발표코드: **ORGN.P-700**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Rate-Equilibria Relationships for Hydride Transfer Reactions of Benzimidazole Compounds with 10-Methylacridinium Ion

한인숙* 정은정[1]

강원대학교 과학교육학부 [1]강원대학교 화학과

The rate and equilibrium constants for the reactions of 3-methyl-2-phenyl-5-substitutedbenzimiazoline, (BIH: CH3, H, Cl) with 10-methylacridinium ion have been measured spectrophotometrically in 2-propanol-H2O (4 : 1, v/v) at 25 + 0.1 oC. The rate constants for these reactions are linearly correlated with the Hammett parameters. The primary kinetic deuterium isotope effect for the reactions of 3-methyl-2-phenyl-5-substitutedbenzimidiazoline-d with 10-methylacridinium ion have also been measured to give values of a range from 4.0 to 5.0. These results will be discussed in terms of mechanism and compared with those of other hydride transfer reactions with NADH analogues

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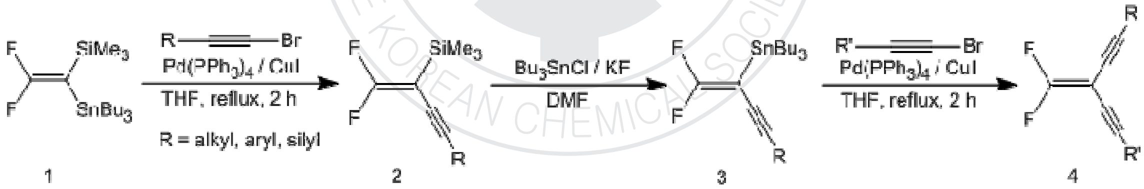
발표분야: 유기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthetic approach to novel 1,1-difluoroendiynes

정예림 김호영 정인화[1,*]

연세대학교 화학과 [1]연세대학교 화학및의화학과

Alkynylation of 2,2-difluoro-1-trimethylsilylstannane **1** with alkynyl bromides in the presence of 10 mol% Pd(PPh_3)$_4$ and CuI in THF at reflux temperature for 2 h provided the 1,1-difluoro-2-trimethylsilylenynes **2** in good yields. Treatment of **2** with Bu_3SnCl and KF in DMF resulted in the formation of tributylstannylated enynes **3**. Further alkynylation of **3** with alkynyl bromides under the same reaction condition afforded 1,1-difluoroendiynes **4** in moderate yields.



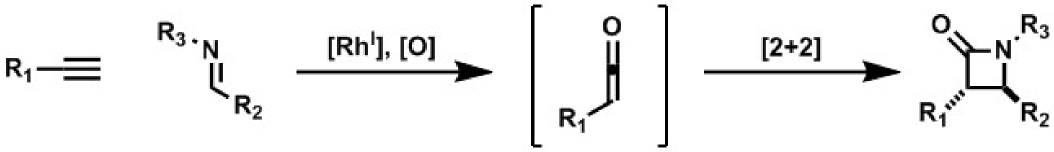
일시: 2014년 4월 16~18일(수~금) 3일간
장소: 일산KINTEX
발표코드: **ORGN.P-702**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Rhodium(I)-Catalyzed Oxygenative [2+2] Cycloaddition Reaction of Terminal Alkynes with Imines for the Synthesis of β-Lactams

노상원 김인수 이동길 이철범*

서울대학교 화학부

Metal-Vinylidene complex exhibit interesting reactivities due to electrophilic nature on the α-carbon of the metal canter and have been used as catalytic intermediates in a variety of reactions of terminal alkynes. Recently, our group reported rhodium(I)-catalyzed oxygenative addition reaction which forms carboxylic acid derivatives from terminal alkynes via a ketene intermediate generated by oxidation of a metal-vinylidene complex. In an ongoing effort to utilize the process, we discovered that the ketene can undergoe a staudinger reaction with imines to give β?lactam products.Herein, we present our results of Rh(I)-vinylidene mediated oxygenative [2+2] cycloaddition of terminal alkynes with various imines giving β?lactam products in good to excellent yields.



up to 96% yield

R_1, R_2 = aryl, alkenyl, alkyl
R_3 = aryl, alkyl, allyl, benzyl

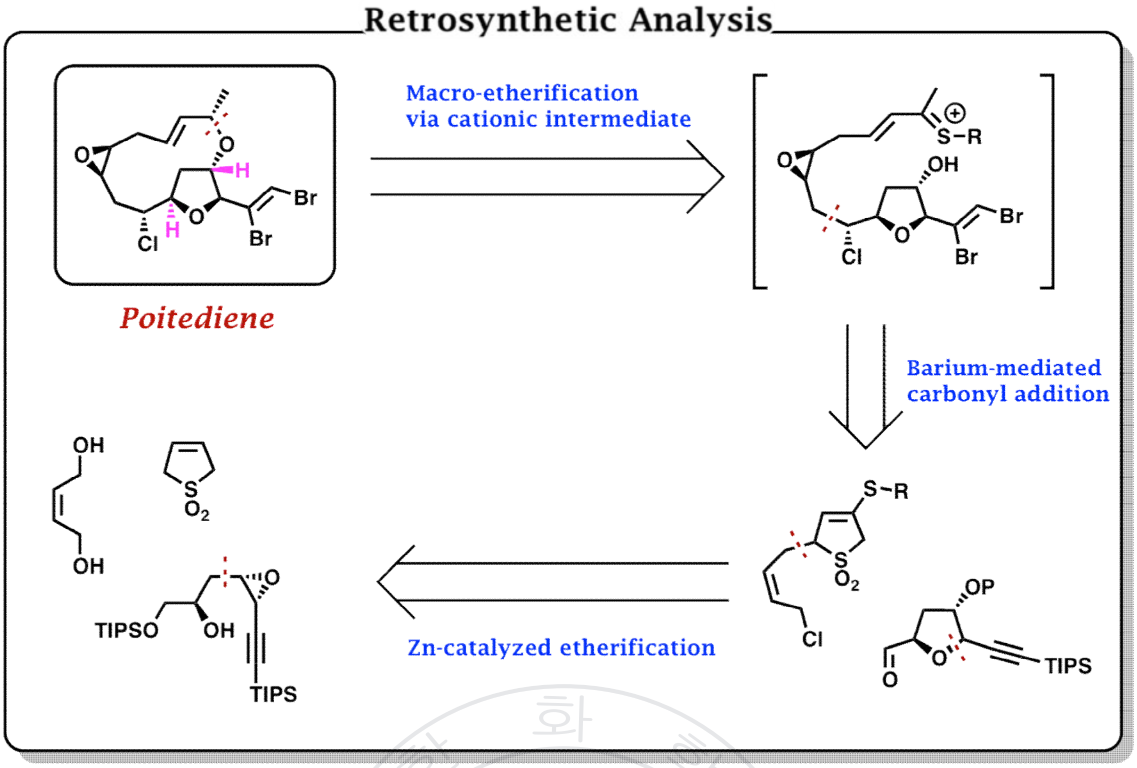
일시: 2014년 4월 16~18일(수~금) 3일간
장소: 일산KINTEX
발표코드: **ORGN.P-703**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Studies toward the Total Synthesis of Poitediene

김선우 **Sinae Kim[1] Robert Matunas[1]** 이철범[*]

서울대학교 화학부 [1]Princeton University, U.S.A.

We present here a novel approach to the enantioselective total synthesis of poitediene, a metabolite of red algae possessing the unique “in-out” bridged cyclic structure. We expect that its highly strained 12-membered macrocyclic ether is constructed from a hetero atom-stabilized carbocation intermediate. The oxolane core was built from epoxy alcohol by zinc-catalyzed etherification, which was a newly founded condition in our group. Described in this poster are the details of our synthetic route that provides efficient access to the highly functionalized 2,12- dioxabicyclo[9.2.1]tetradecane system.


Retrosynthetic Analysis
Poitediene
Macro-etherification
via cationic intermediate
Barium-mediated
carbonyl addition
Zn-catalyzed etherification
O
O
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H
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O2
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TIPS

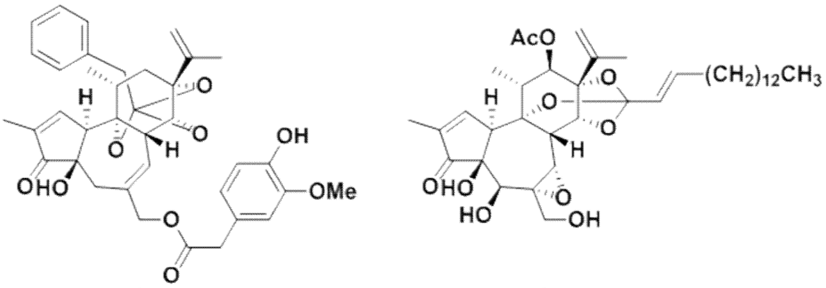
일시: 2014년 4월 16~18일(수~금) 3일간
장소: 일산KINTEX
발표코드: **ORGN.P-704**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

The synthetic study of daphnane family natural products: formation of 7,6-membered ring structure

<u>김영습</u> 배애님[1] 이재균[2] 조용서[1,*] 민선준[3,*]

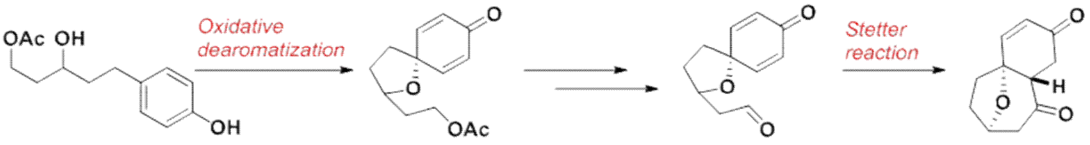
과학기술연합대학원대학교(UST) 생체분자과학 [1]한국과학기술연구원(KIST) 생체과학연구본부 [2]한국과학기술연구원(KIST) 케모인포매틱스연구단 [3]한국과학기술연구원(KIST) 뇌의약연구단

The daphnane family natural products exhibit a broad range of activities such as anti-leukemic, skin irritant, neurotrophic, anti-hyperglycemic, anti-fertility and pesticide. Most of the daphnane products constitute 5,7,6-membered ring core structure with quaternary oxygen and orthoester in 7, 6-membered ring junction (Figure 1). Although the structure of such daphnanes is highly complex, they are still extremely challenging synthetic targets due to their potent biological activities.In our laboratories, we have endeavored to identify an approach that would allow for rapid access to the 7,6-membered ring core structure 6 having trans-fused ring juncture. The synthesis commenced from commercial available ethyl acetate and acrolein. After Heck reaction with 4-iodoanisole and aldol product, 3-hydroxy-5-(4-hydroxyphenyl)pentyl acetate 3 was converted into spirocyclic compound 4 by oxidative dearomatization. The resulting spirocycle 5 was installed the 7-membered ring using Stetter reaction as key step (Scheme 1). This synthesis will allow for the introduction of oxygen in 7,6-membered ring core structure having trans-fused ring juncture and the preparation of orthoester in synthetic analogues of daphnane.



1 2

Figure 1. The structure of daphnane family: Resiniferatoxin (**1**) and Kirkinine (**2**)



3 4 5 6

Scheme 1. The synthesis of 7, 6-membered ring core structure

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장소: 일산KINTEX
발표코드: **ORGN.P-705**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Poly(9-(3-Vinyl-phenyl)-phenanthrene)을 기반으로 한 새로운 Blue Emitting polymer의 합성과 발광 특성

양가람 박종욱*

가톨릭대학교 화학과

Polymer light-emitting diodes(PLEDs)는 flat-panel display 와 조명과 같은 다양한 분야에 응용될 수 있어 학계 및 산업 분야에서 주목을 받아 왔다. 이 논문에서 우리는 Phenanthrene 을 기반으로 한 새로운 blue emitting polymer 인 poly(9-(3-Vinyl-phenyl)-phenanthrene)(PVPP)를 합성했다. NMR data 로부터 vinyl group proton 들이 사라지고, polymer 의 특성에 의해서 aromatic proton 들이 broad 한 proton peak 들을 보였다.

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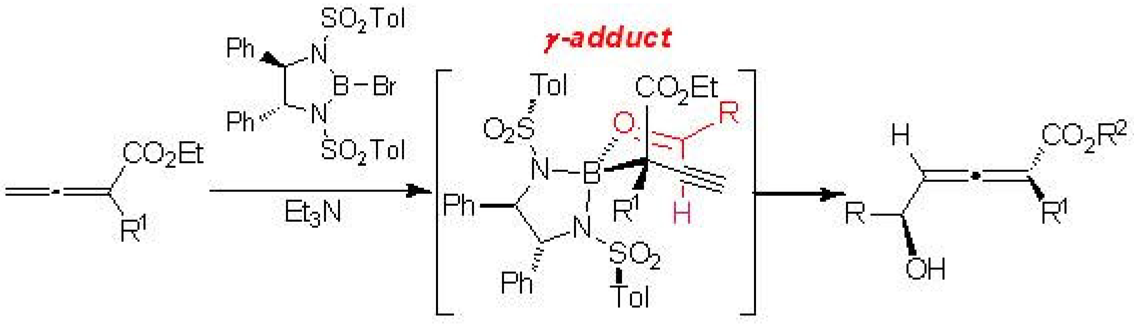
발표코드: **ORGN.P-706**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

A Construction of Center and Axis Chirality through Aldol Reaction of Allenoates: Formation of Unprecedented Gamma Addition Products

방지윤 정서우 이은혜 유찬모*

성균관대학교 화학과

The availability of efficient synthetic methods for achieving absolute stereoselectivity in the production of enantiomerically pure compounds is of considerable current interest in synthetic chemistry. Recently, we have developed a new adol method of the allenoate process in forming 2-hydroxy allenolate in high levels of enantioselectivity. In light of this progress, we turned our attention to achieve chiral quaternary stereocenter. After conversion of alleneoate to the borone enolate in the presence of chiral bromoborane complex followed by an addition of aldehyde resulted in the formation of gamma addition aldol adduct in high levels of diastereoselectivity. We would like to present herein the scope of reaction, stereoselectivity, and its applications.



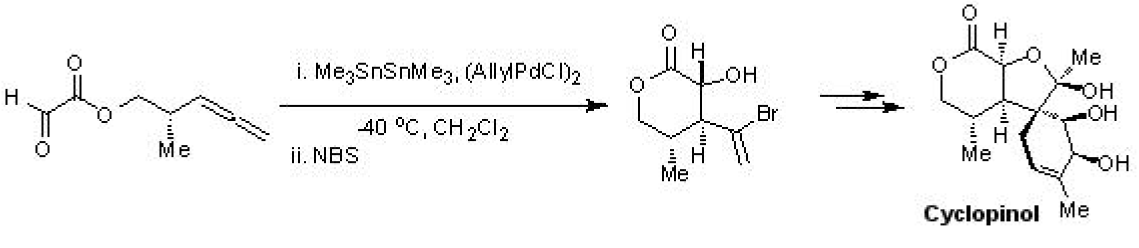
일시: 2014년 4월 16~18일(수~금) 3일간
장소: 일산KINTEX
발표코드: **ORGN.P-707**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

A New Carbocyclization of Allenyl-glyoxylates via Palladium Catalysis through Three-component Assembly: Synthesis of Cyclopinol

오세민 김나나 유찬모*

성균관대학교 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. In this purpose, we have recently disclosed our investigations on the transition metal catalyzed intramolecular allylic transfer reactions to afford cyclic compounds in high levels of stereoselectivity. 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 cyclopinol, a family of cyclocalopins.



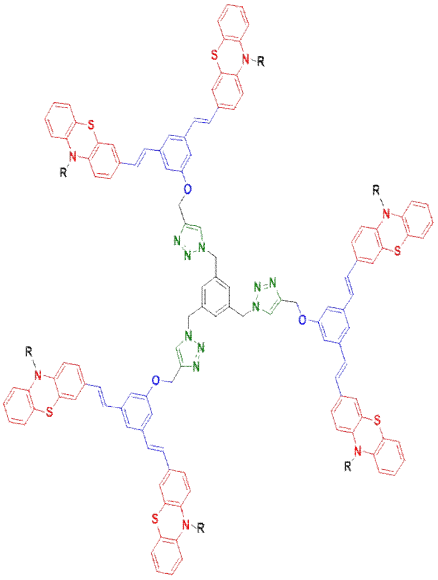
일시: 2014년 4월 16~18일(수~금) 3일간
장소: 일산KINTEX
발표코드: **ORGN.P-708**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Phenothiazine dendrimers: Synthesis, characterization and their application in Dye Sensitized Solar Cells

CHINNADURAISATHEESHKUMAR 정동철 송선구 송창식*

성균관대학교 화학과

Dendrimers are perfect monodisperse macromolecules with a regular and highly branched three-dimensional architecture.1-3 Dendrimers are one of the most exciting class of macromolecules that have sparked significant interest in recent years from synthetic, structural and functional points of view. The properties of dendrimers like solubility, viscosity and thermal behaviour are dominated by the nature of the surface or end group. Phenothiazine based dendrimers finds applications in electronics and optoelectronics including light-emitting diodes, thin film transistors and dye sensitized solar cells. Click chemistry4 refers to the 1, 3-dipolar cyclo addition of azide to acetylenic in the presence of $CuSO_4.5H_2O$, NaAsc in a 1:1 solvent ratio of THF and H_2O. The present investigation mainly focuses on the design and synthesis of dendrimers using phenothiazine at the end-group through Horner-Wadsworth-Emmons and click reactions. Herein, we wish to present various type of dendrons and dendrimers with phenothiazine as surface group and discuss their photophysical properties and usage in Dye Sensitized Solar Cells (DSSCs).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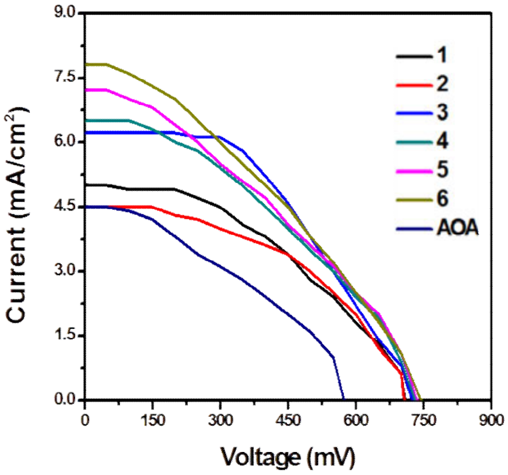

Current (mA/cm^2)
Voltage (mV)
9.0
7.5
6.0
4.5
3.0
1.5
0.0
0
150
300
450
600
750
900
1
2
3
4
5
6
AOA

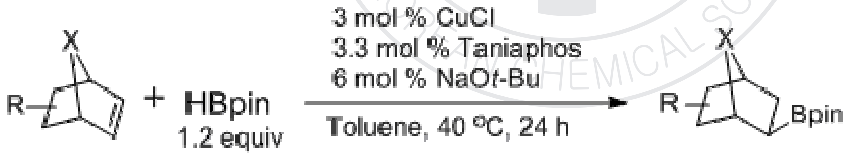
일시: 2014년 4월 16~18일(수~금) 3일간
장소: 일산KINTEX
발표코드: **ORGN.P-709**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

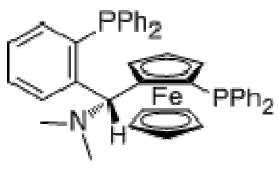
Cu-Catalyzed Enantioselective Hydroboration of Strained Bicyclic Alkenes

이병윤 이우림 윤재숙*

성균관대학교 화학과

Asymmetric hydroboration of strained bicyclic alkenes is a very interesting reaction. Hydroboration reactions using Pd-, Rh-, Ir-catalysts showed high enantioselectivity in general alkenes, but they resulted in low enantioselectivities for strained systems.In this study, we investigated copper-catalyzed asymmetric hydroboration of strained bicyclic alkenes by using pinacolborane. The resulting boron compounds could be obtained with high enantiomerical purity.





(R,R)-Taniaphos

일시: 2014년 4월 16~18일(수~금) 3일간
장소: 일산KINTEX
발표코드: **ORGN.P-710**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Efficient Syntheses of Ieodomycin B and Its Analogs

설재희 이종석[1,*] 박솔[2] 이희승[3] 이연주[4] 신희재[5]

한양대학교 응용화학과 [1]한국해양과학기술원 해외생물자원 연구센터 [2]과학기술연합대학원대학교(UST) 해양생명공학과 [3]한국해양연구원 해양천연물연구실 [4]한국해양연구원 해양바이오센터 [5]한국해양연구원 천연물연구실

Marine-derived microorganisms are increasingly recognized as the true metabolic sources of marine natural products with therapeutic and pharmaceutical importance.Ieodomycin B is among the four unsaturated fatty acids discovered from bioassay-guided isolation of the culture extract of a marine Bacillus sp. 09ID194 obtained from sediment in Ieodo, Republic of Korea's southern reef. As part of our on-going program for the discovery of bioactive substances from marine organisms and the subsequent construct of marine natural product-based small molecular library, it was an urgent need to develop an efficient synthesis of ieodomycins for material supply. Herein we describe the efficient syntheses of ieodomycin B and its analogs using (1) Ti-catalyzed asymmetric allylation of an aldehyde. (2) Stereoselective iodolactonization. (3) Completion of the synthesis of ieodomycin B and its analogs by coupling of various allyl tributyltin compounds with the corresponding iodolactone.

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

Theoretical Investigation on the Destiny of $PdCl_2(CH_3CN)_2$ Catalyst Precursor in the Presence of Phosphine Ligands; Pd(II) Reduction to Pd(0)? Or Simple Ligand Substitution?

박지은 강윤경*

상명대학교 화학과

Palladium catalyzed reactions are widely used in modern organic chemistry. $PdCl_2(CH_3CN)_2$ is a common catalyst precursor for many Pd-catalyzed reactions, usually being used in combination with phosphine ligand. In spite of its popularity, the detailed information regarding the transformation behavior of this precursor molecule to the active catalyst species has not been reported. Here, we present the reaction energetics of $PdCl_2(CH_3CN)_2$ in the presence of triphenyl phosphine ligand calculated by using density functional theory. The effect of oxygen donor solvent is also considered explicitly. The results show that the ligand substitution reaction occurs dissociatively, which is against the textbook theory. Sequential substitutions of two CH_3CN ligands with two triphenylphosphines are mostly favorable. Substitutions of chloride ions or a reductive elimination of two chlorine atoms are physically unattainable, implying that Pd(II) cannot be reduced to Pd(0) under such a reaction condition. Reduction of Pd(II) to Pd(0) is possible when hydroxide is present by forming phosphine oxide.

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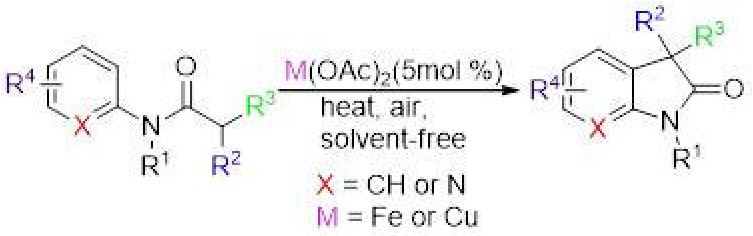
발표코드: **ORGN.P-712**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Solvent-Free C-C bond Formation of Oxindole Derivatives in Air

손세인 송호림[1] 이원구[1,*] 하현준[2,*]

서강대학교 화학 [1]서강대학교 화학과 [2]한국외국어대학교 화학과

Oxindole derivatives are used for a wide range of applications including traditional herbal medicine like Horsfiline1, anti-inflammatory agents2, molecular probes for pharmacological research3 and radical olefination reactions for the preparations of biologically interesting compounds4. Therefore, much effort has been made to develop efficient methods for preparing these molecules including famous name reactions such as Buchwald?Hartwig amination which require pre-functionalization by using halogen-substituted material 5-10. Previous experiments use halogen substituted materials because it is difficult to obtain oxindole derivatives without pre-functionalization by halogen which activates the ring at the initiation of the reaction. We recently developed methodology which does not need pre-functionalization with halogens, making this reaction environmentally friendly. While we studied CH activation, we realized that the organic solvent was not the important reagent for obtaining products. Therefore, we synthesized oxindole derivatives without organic solvent or extra additives. The required oxidant in this methodology is oxygen from air, and the reaction does not require an inert atmosphere. We used air to oxidize the intermediate and the method is appropriate for the preparation of pyridine derivatives which are rarely prepared through C-H activation.



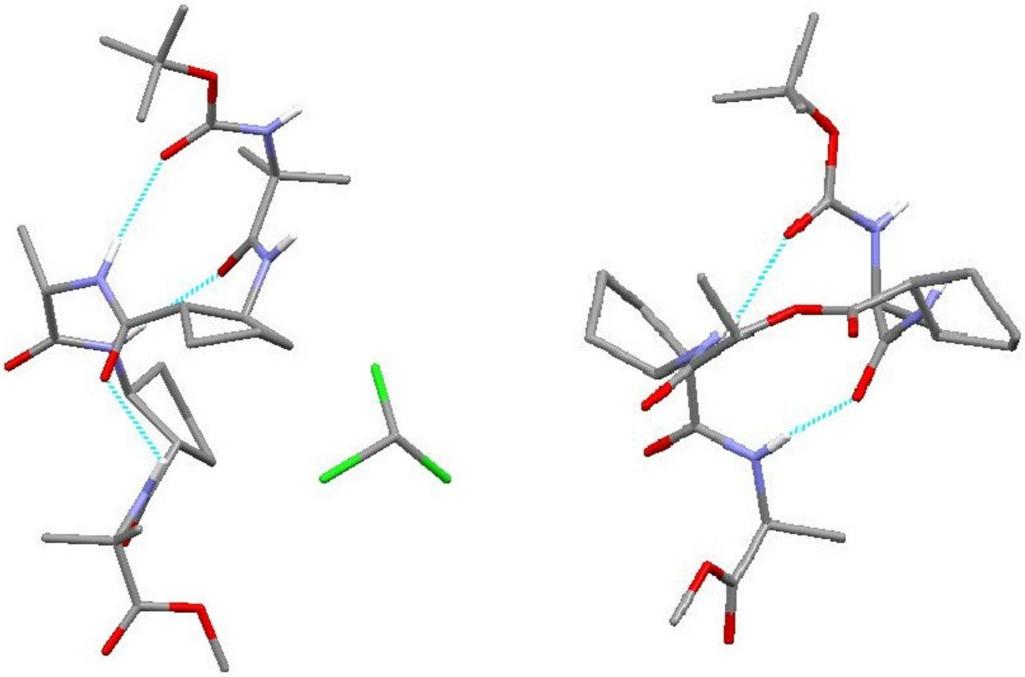
일시: 2014년 4월 16~18일(수~금) 3일간
장소: 일산KINTEX
발표코드: **ORGN.P-713**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis and Conformational Study of Unnatural Peptides Containing Lactic-acid

이재연 장근혁 강필재 최수혁*

연세대학교 화학과

In the past decade, increasing work has been devoted to the study of foldamers that describe any polymer with a strong tendency to adopt specific compact conformation.Here, We will study depsipeptides that are oligomers containing hydroxy acid residues. We wondered what the effect of transforming NH-group into ester group in alternating 1:1 α/β-peptide containing ACPC would be. We designed α/β-depsipeptides backbone containing lactic acid to observe new helical pattern.



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장소: 일산KINTEX
발표코드: **ORGN.P-714**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis of Bi-naphthalene-based Low Band Gap Polymers for Polymer Solar Cells Application

박성민 김희원 V. Tamilavan 현명호*

부산대학교 화학과

Polymer solar cells (PSCs) have attracted a great deal of attention because of the low-cost, light-weight, and mechanical flexibility. In polymer BHJ solar cells, conjugated polymers are used as electron donor (D) materials and fullerene derivative, [6,6]-phenyl-C71-butyric acid methyl ester (PC71BM), is usually used as electron acceptor (A) material. At present, diketopyrrolopyrrole (DKPP) based electron accepting monomer is widely used to develop new donor-acceptor polymers for PSCs due to their high solar energy to electrical energy conversion efficiency. As an effort to utilize DKPP based polymers further in PSC applica-tions, we copolymerized electron deficient DKPP unit with electron rich non-planar binaphthalene (BN) and N-bridged binaphthalene (BNN) units to afford polymers P(BN-DKPP) and P(BNN-DKPP), respectively. Both polymers showed broad absorption band from 300 nm to 750 nm with optical onset at 1.76 nm and 1.72 nm, respectively. The HOMO energy level of P(BNN-DKPP) was found to be deeper than that of P(BN-DKPP) and located at -5.43 eV and -5.26 eV, respectively. The LUMO energy level of the polymers was estimated to be -3.71 eV and -3.50 eV, respectively. The suitable energy levels and broad absorption ability of polymers P(BN-DKPP) and P(BNN-DKPP) induced us to apply them in PSCs application. The study concerning the pho-tovoltaic properties of new polymers P(BN-DKPP) and P(BNN-DKPP) are under progress.

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발표종류: 포스터, 발표일시: 수 16:00~19:00

Imidazolium Iodide Salts as Organic Ionic Plastic Crystals

이민재

군산대학교 화학과

A series of alkylene 1,2-bis[N-(N'-alkylimidazolium)] iodide salts was synthesized and characterized. The new imidazolium iodide salts show multiple solid-solid phase transitions below their melting temperatures. The phase transition temperatures are dependent on the N-substituted alkyl chain length of the imidazolium moiety. Only the C_2 (ethylene) connected bisimidazolium salts show the multiple solid-solid phase transitions and the other salts with a longer bridge only show a melting behavior with a temperature raise. The new imidazolium iodide salts could be called organic ionic plastic crystals because of their multiple solid-solid phase transitions and relatively low ΔS_f values. These new imidazolium iodide salts could be applied to the solid-electrolytes of dye-sensitized solar cell and other electrochemistry areas which use organic iodide salts.

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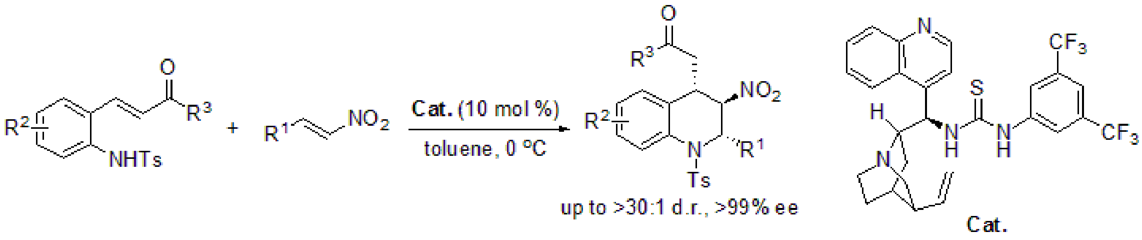
Asymmetric Domino Aza-Michael/Michael Reaction of o-N-Protected Aminophenyl α,β-Unsaturated Ketones with Nitroalkenes: Construction of Chiral Highly Functionalized Tetrahydroquinolines

김신애 이요나 김성곤*

경기대학교 화학과

The diastereo- and enantioselective synthesis of 2,3,4-trisubstituted tetrahydroquinolines has been developed through organocatalytic domino aza-Michael/Michael reaction of o-N-tosylaminophenyl α,β-unsaturated ketones with nitroalkenes. This useful and simple domino process afforded diverse highly functionalized tetrahydroquinolines, some of which are not easily accessible using other methodologies, in good yields and with excellent diastereo- and enantioselectivities (up to >30:1 d.r., >99% ee).



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발표코드: **ORGN.P-717**
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발표종류: 포스터, 발표일시: 수 16:00~19:00

Palladium-catalyzed arylation of thiole and aryl bromide with N-amido imidazolium salts as ligands

노지은 임정아 이선우*

전남대학교 화학과

We developed the method for the synthesis of diaryl sulfide via palladium catalyzed c-s bond cross coupling with N-amido imidazolium salts as ligands. The best combination for the coupling with aryl bromides was N-amido imidazolium salt 2 and NaHMDS, and that for the coupling with aryl iodides was N-amido imidazolium salt 1 and KOtBu. The coupling reactions were conducted in the presence of Pd(OAc)2 (1 mol%) in DMSO at 80 o C for 12 h.

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발표종류: 포스터, 발표일시: 수 16:00~19:00

An Efficient and Reusable Palladium Catalyst for Reduction of Nitroaromatic Compounds and Aryl Halides

민홍근 이선우*

전남대학교 화학과

We developed an efficient reduction method of nitroaromatic compounds and aryl halides to produce highly active palladium nanopaticle in poly styrene (PS-Pd). The catalyst is recovered quantitatively by simple filteration and was reused for several times with consistent activity. The optimized condition is that 10 mol% of PS-Pd, 1.5 equivalent K_3PO_4, the excess amount of cyclohexanol was reacted in DMF at 150℃ for 24 hours.

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

The Synthesis of Propargylamines by the Additive-Free Three Component Reaction of Alkyne Carboxylic Acids, Paraformaldehyde and Amines

박경호 이선우* 이기복

전남대학교 화학과

We successfully synthesized propargylamines with alkyne carboxy acids, paraformaldehyde and amines without any additives. On the other hand, previous synthetic routes to the compound from terminal alkynes required metal catalyst such as copper, gold, silver, iridium, indium, iron and zinc. This strength may impact on fine chemical industry. Moreover, The reactions of the molecules combined with alkyne carboxy acid and terminal alkyne showed high selectivity toward alkyne carboxy acid.Reference: K. Park,; Y. Heo,; S. Lee *Org. Lett.* 2013*, 15*, 3322.

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

The One-Step Synthesis of the Conjugated Random Co-Polymers of Poly-(p-phenyleneethynylene)s (PPEs) and poly-(p-phenylenebutadiynylene)s (PPBs)

박경호 이선우*

전남대학교 화학과

We synthesized the conjugated random co-polymers which consist of poly-(*p*-phenyleneethynylene)s (PPEs) and poly-(*p*-phenylenebutadiynylene)s (PPBs) as a core by one-step reaction. This method is economically efficient because the previous methods required a multi-step reaction, such as Sonogashira reaction and de-protection of protected terminal alkyne to convert from the diiodoarene as starting material to diethynylarene before polymerization, and the each step bring out the reaction wastes such as reagents, solvent and catalysts. The origin of the idea for this method based on recent our report, palladium catalyzed decarboxylative coupling reaction of aryl halides with propiolic acid.Reference: T. Vokataa,; M. R. Kumara,; K. Park,; J. H. Moon,; S. Lee *Synlett* 2013, *24,* 1563.

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발표종류: 포스터, 발표일시: 수 16:00~19:00

Development of Fluorescent Chemosensor for Ions with Anthracene Amino Derivative

심남연 남계춘*

전남대학교 화학과

Ions play an important role in a wide range of chemical and biological processes and considerable attention has been focused on the design of host molecules that are able to selectively recognize and sense ion species. Fluorescent chemosensors can be effectively used as a tool to analyze and clarify roles of charged chemical species in living system due to the high sensitivity. Therefore design and synthesis of fluorescent sensors for ions is greatly important for both chemical and biological applications.We developed several anthracene amino derivatives which could play as a fluorescent chemosensors in various photochemical and colorimetric systems. Synthesis and the binding properties for ions with 1H-NMR, UV-vis and fluorescence spectroscopy will be presented

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발표종류: 포스터, 발표일시: 수 16:00~19:00

$Pd(PPh_3)_4$ catalyzed One-Pot Synthesis of the Unsymmetrical Diarylalkynes from Two Different Aryl Bromides and Propiolic Acid

황진일 최진섭 이선우*

전남대학교 화학과

Symmetrical diarylalkynes usually generate under palladium catalyzed reaction from aryl halides and propiolic acid. The control of the undesired symmetrical diarylalkynes is very difficult. So we tried to control symmetrical diarylalkynes and make ideal unsymmetrical diarylalkynes.Palladium catalyzed Sonogashira reaction is the most commonly used method for the arylation of terminal alkynes. Instead of the terminal alkynes, the decarboxylative Sonogashira reaction is used from the alkyne carboxylic acids has several advantages, including a depreciable process for the treatment of the carbon dioxide as a reaction waste released after the complete conversion, and is stable for handling and storage.We found a method of the site selective reaction of propiolic acid with two different aryl bromides combinations using decarboxylative Sonogashira reaction that generate unsymmetrical diarylalkyne products. The method was able to make the desired materials using the temperature. The optimized condition is that aryl bromide (1.0 and 1.2 equiv), propiolic acid (1.2 equiv), $Pd(PPh_3)_4$ (5mol%), DBU (2.4 equiv) were reacted in DMSO at 35 ^{o}C for 24 h and at 90 ^{o}C for 12 h. In conclusion, the method for the synthesis from the Pd-catalyzed Sonogashira reaction with propiolic acid and two different aryl bromides of desired unsymmetrical diarylalkynes has been developed. The various synthesis of two different aryl bromides showed good yields.

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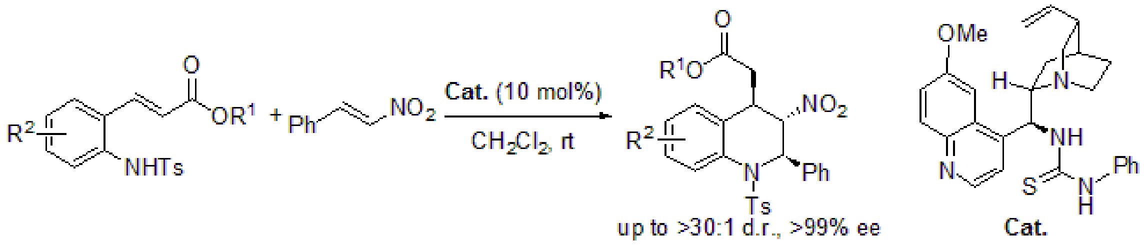
발표종류: 포스터, 발표일시: 수 16:00~19:00

One-Pot Catalytic Enantioselective Synthesis of tetrahydroquinolines via a Aza-Michael/Michael Cascade Reactions of o-N-Protected Aminophenyl α,β-Unsaturated Esters with Nitroalkenes

강기태 <u>김철웅</u>[1] 김성곤[2,*]

성균관대학교 화학과 [1]경기대학교 화학 [2]경기대학교 화학과

The synthetic methodology of chiral highly functionalized tetrahydroquinolines has been developed based on the organocatalytic enantioselective aza-Michael/Michael cascade reaction of of o-N-protected aminophenyl α,β-unsaturated esters with nitroalkenes. The asymmetric catalytic reactions using cinchona alkaloid-derived thiourea as an organocatalyst activating the nitroalkene through hydrogen-bonding interactions have produced the desired products in good yields and with excellent diastereo- and enantioselectivities (up to >30:1 d.r., >99% ee).



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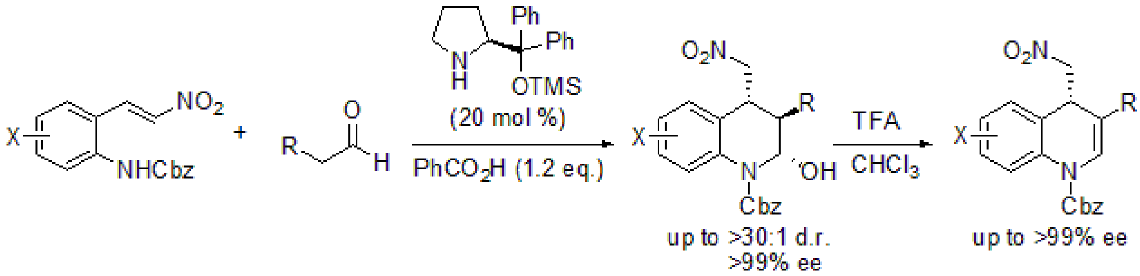
발표코드: **ORGN.P-724**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Organocatalytic Asymmetric Cascade Reactions of Aldehyde to 2-Aminonitrostyrene: Facile Synthesis of Chiral Tetrahydroquinolines & Dihydroquinolines

이요나 김성곤*

경기대학교 화학과

A organocatalytic enantioselective Michael addition?cyclization reaction of normal aldehydes with 2-aminonitrostyrenes has been established using a diphenylprolinol TMS ether as an organocatalyst. The reaction afforded the corresponding 2,3,4-trisubstituted tetrahydroquinolines in good yields and with high levels of stereoselectivities (up to >30:1 d.r., >99% ee). Chiral 4-substituted dihydroquinolines derivatives have been readily obtained through the subsequent transformation of these products.



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

Regioselective Synthesis of Isocoumarins and Pthalides from 2-Iodobenzoic Acids and Alkynes

IRUDAYANATHANFRANCISMARIARAJ 이선우*

전남대학교 화학과

The coupling reactions of 2-iodobenzoic acids and alkynes such as terminal acetylene, alkynyl carboxylic acids, and trimethylsilyl acetylenes selectively afforded isocoumarins and phthalides in the presence of CuI as a catalyst. At 100°C , the 6-endo-dig product, isocoumarin, was formed and at 25°C the 5-exo-dig product, phthalide, was formed as a major product. A mechanism is suggested in which the formation of 2-alkynyl benzoic acid as an intermediate via Sonogashira-type coupling was ruled out in the reaction pathway.

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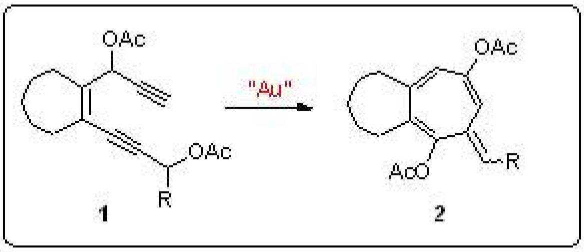
발표분야: 유기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

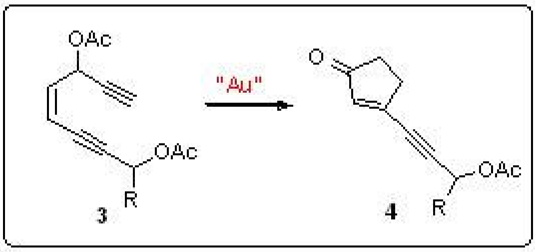
Gold-catalyzed Cyclization of 3-(3-oxocyclopent-1-enyl)prop-2-ynyl acetate

유진 김소영 오부근 오창호*

한양대학교 화학과

Transition metal catalyzed C-C bond formation has been investigated by numerous organic chemists and it has been a powerful tool in synthetic organic chemistry. Because of alkynophilicity of gold, many scientists were attracted by this interesting field. Our group reported a novel gold-catalyzed transformation of 1 which involving two propargylic carboxcylate. This substrate was transformed into the corresponding benzo[7]annulene product 2. Based on this fruitful research, we prepared an acyclic propargylic carboxylates 3. Unexpectedly, after treating with a gold catalyst, it was formed the corresponding cyclopentanone product 4.





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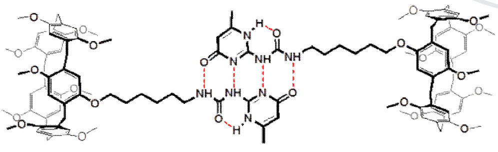
발표코드: **ORGN.P-727**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Self-assembled supramolecular nanostructures of ureido-4[1H]-pyrimidonyl copillar[5]arenes and pyridinium bridges

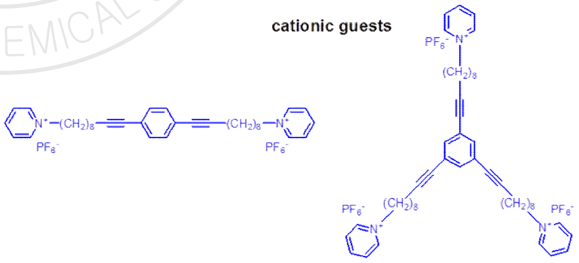
이재철 박연실 백경수*

숭실대학교 화학과

Copillar[5]arene **1** mono-substituted with ureido-4[1H]-pyrimidone itself forms stable dimer **1_2** by quadruple hydrogen bonds in nonpolar solvent, and dimer **1_2** can self-assemble into supramolecular nanostructures through cation-π interactions when cationic bridging guests are present. Self-assembled supramolecules can control their size and shape by the sequence of addition of guests and copillar[5]arene **1**. The characteristics of these self-assembled supramolecular nanostructures were studied by ^{1}H NMR and atomic force microscopy (AFM).



1_2


cationic guests

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Hantzsch ester and S-benzyl isothiouronium iodide as efficient reagents combination for the direct reductive amination of aldehydes and the reduction of conjugated nitroalkenes into nitroalkanes

이하늬 김택현[1,*]

전남대학교 신화학소재공학과 [1]전남대학교 응용화학공학부 광바이오사업단

Hantzsch ester, a well-known model compound of co-enzyme nicotinamide adenine dinucleotide(NADH), has been found to be an attractive reducing agent for a variety of useful organic transformations, because they overcome the metal residual problem encountered with traditional reductive reagents such as hydrogen gas/metal and metal hydrides. Isothiouronium salts have been explored recently as a new class of hydrogen-bonding subunit as thiourea. Isothiouronium group has more advantages: it enhances the NH acidity compared to the corresponding thiourea. Herein, we will discuss the effect of S-benzyl isothiouronium salts as an activator in the reductive amination of aldehydes and the reduction of conjugated nitroalkenes into nitroalkanes from the viewpoint of the reaction rate depending on the counter anion of these salts.

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발표종류: 포스터, 발표일시: 수 16:00~19:00

Visual detection of carbon dioxide and pathogenic bacteria based on imidazolium-functionalized polydiacetylenes

이송이 윤주영[1,*]

이화여자대학교 화학나노과학과 [1]이화여자대학교 화학·나노과학과

Polydiacetylenes (PDAs) exhibit a characteristic blue-to-red phase transition that can be triggered when stimuli disrupt the effective polymer conjugation length, typically by inducing a change in the preferred backbone conformation. This unique property of PDAs has been adopted in the development of various chemosensors.Our first sensor design based on imidazolium relies on the reaction of carbon dioxide with alkylamines tethered to the imidazolium PDA to induce the blue-to-red phase change. In the presence of an added base, carbamic acid salts that partially neutralize the polymer's positive charges are generated, affecting the solvation of the side-chains and resulting in changes to the backbone conformation. The signal change is maximized by the covalent linking of the carbamates to prevent their diffusion away from the polymer. Our second imidazolium-based conjugated polydiacetylenes show not only significant antibacterial efficacy and but also distinct colorimetric change from blue to red with pathogenic bacteria. In this study, we prepared PDA (polydiacetylene) solutions (PDAs) derived from imidazolium monomers and imidazole monomers to instantaneously detect and also rapidly kill most of bacterial cells. Transmission electron microscopy (TEM) showed considerable changes in the bacterial cell membranes upon PDAs treatment. The present study suggests that this PDAs solution has great potential to be used as probe-killer for various pathogenic strains including MRSA (methicillin-resistant Staphylococcus aureus) and ESBL-EC (extended spectrum β-lactamase producing- Escherichia coli)

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발표종류: 포스터, 발표일시: 수 16:00~19:00

Selective fluorescent Probes for Biological Thiols and Bioimaging in live cells and Mice

김다빈 이다영[1] 신인재[2,*] 윤주영[3,*]

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Detection of biothiols has been studied in biological and biomedical applications. Because biological thiols including glutathione (GSH), cysteine (Cys), homocysteine (Hcy) play a crucial role in physiological and pathological process, perception of biothiols provides crucial information about physiological process.In these reasons, the selective fluorescent sensors were designed, developed, and utilized for observation of biothiols in live cells and mice. In the presence of biothiols, such and glutathione (GSH), cysteine (Cys), homocysteine (Hcy), probes display fluorescent enhancement.

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A rational approach to enhance thermochromic property of polydiacetylenes (PDAs) and its theoretical simulations

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The new type of PDA, Bis-PDA-Ph, which contains two PDA moieties and p-phenylene group, was developed. In the preparation of polymer, DA monomer, Bis-PCDA-Ph, used in this study. And than, PDA-embedded electrospun fibers were prepared by Bis-PDA-Ph and poly(ethylene oxide)(PEO) solution. The new electrospun fibers, which is built with Bis-PDA-Ph, undergo a reversible color transition between 20-120 ℃. That is the largest range observed thus far for PDAs. These newly designed fibers were observed to display excellent thermochromic reversibility as a consequence of the unique hydrophobic interctions between alkyl chains. The ene-yne conjugated backbone of the New PDA is rigid, so the measured orientation correlation function, C1 changes only slightly. The colorimetric change, blue to red and red to blue, indicated that Bis-PDA-Ph-embedded fibers are fully reversible. Furthermore, a unique broad range of temperature can also affect this phenomenon.

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Thiazolothiazole derivatives based Fluorescent Colorimetric chemosensor for Cu^{2+} via unique radical formation

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New thiazolothiazole-based Cu^{2+} colorimetric and fluorescent sensors are reported. A highly selective color change and selective fluorescent quenching effect were observed upon the addition of Cu2+. The simple thiazolothiazole derivatives 1, 2 and 3 can act as a Cu^{2+} selective colorimetric and fluorescent sensor via unique radical formation.Electrochemical and electron paramagnetic resonance data proved the formation of an organic radical.

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Fluorescent probe for RNA detection based on bispyrene

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RNA detection and analysis has great importance, but few examples of RNA detection can be found. Herein, we synthesized a novel fluorescent probe based on bispyrene with high selectivity and sensitivity for RNA detection in aqueous solution at pH 7.4. This probe can be used for fluorescence imaging of RNA in living cells, so it is suited for biological RNA analysis.Reference1. Y. Liu, E. J. Jun, G. Kim, A-R. Lee, J-H. Lee, J. Yoon, Chem. Commun., 2014, 50, 2505-2507.

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Asymmetric alkylation reaction using benzene based 2-imidazolidinone as chiral auxiliary

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Asymmetric alkylation reaction using chiral auxiliaries is a general method for the formation of carbon-carbon bonds in organic synthesis. We develop more effective chiral auxiliary, allowing two diastereoselective reactions to occur simultaneously in the same sense of asymmetric induction on a single substrate molecule. The study is to use symmetrical benzene based 2-imidazolidinone having double asymmetric alkylation reaction center. In addition, we will also discuss the recovery and reuse of this chiral auxiliary.

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Non-biofouling efficacy of polysaccharide on glass surfaces

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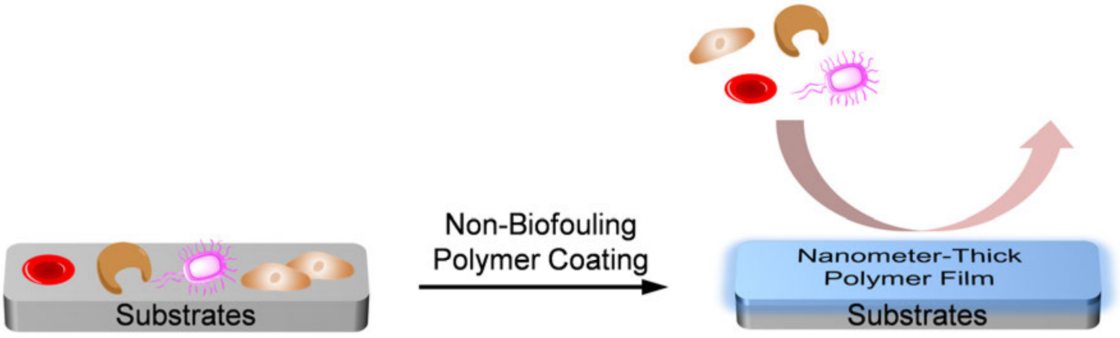
Biofouling, the deterioration of device and surface function resulting from the accumulation of bioentities (e.g., proteins, cells, and bacteria), is an important issue in a wide range of areas such as biomedical devices, biosensors, medical implants, drug delivery carriers, food industry, marine equipment, and water purification systems. To minimize the biofouling, it is prerequisite to introduce functionalities on solid surfaces, including metals and polymers, which not only minimize the unwanted, non-specific adsorption of bioentities, but also improve the device function. The formation of non-biofouling polymer on the surfaces is one of the best methods to reduce the non-specific adsorption. Thus, we coated polysaccharide as a non-biofouling polymer onto glass surface, and then functionalized the polysaccharide-coated glass through surface organic reactions. The non-biofouling efficacy of the polymer was monitored by fluorescence analysis, such as a microarray scanner.



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Highly Efficient Multi-chromophore Emitters System Based on Phenanthrene Moiety for OLEDs

강석우 박종욱*

가톨릭대학교 화학과

We describe two blue emission materials based on a new type of mulit-chromophore concept. TAnDAP, TAnPDAP were synthesized through boronylation and Suzuki coupling reactions. One of multi-chromophore system derivatives, TAnDAP, exhibited an PLmax value of 421nm and The other material TAnPDAP exhibited an PLmax 433nm in Solution. The multi-chromophore materials had narrower PL in solution But broad PL spectra in Film and better thermal properties than the single core chromophore materials.

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Charge Transfer Based Colorimetric Detection of Silver Ion

한승철 윤성희 이재욱*

동아대학교 화학과

Chemosensors are the molecules of abiotic origin that bind selectively and reversibly with the analyte with concomitant change in one or more properties of the system. The recognition and signaling of ionic and neutral species of varying complexity is one of the most intensively studied areas of contemporary supramolecular chemistry. Among different types of chemosensors, colorimetric/chromogenic chemosensors are especially attractive because the guest determination can be carried out by the naked eye, without the use of expensive equipment and they also find direct applications in the development of optodes and disposable dip-stick arrays based on absorption changes. Although molecules containing an electron donor and an electron acceptor linked by a spacer have also been studied extensively in conjunction with the development of stable intramolecular CT complex, to the best of our knowledge, there is no report to sense the analyte using molecules containing an electron donor and an electron acceptor linked by a spacer. In continuation with our research on the self-assembling supramolecular systems via donor?acceptor interactions, we were intrigued to apply this interaction for signaling of ionic species. Herein we report on the design and synthesis of U-shape molecule which is linked by oligoethylene glycols (OEGs) between an electron-deficient (methyl viologen; MV2+) and an electron-rich (2,6-dialkoxynaphthalene; Np) units and their application on sensing metal ion.

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Asymmetric synthesis of homoallylic amines having quaternary carbon centers via allylic addition to hydrazones

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There has been great interest in developing methods for asymmetric nucleophilic allylic addition of organometallic reagents to imine derivatives. Homoallylic amines containing quaternary carbon centers are valuable compounds which are used as building blocks for preparing biologically active molecules. However, controlling the stereochemistry of quaternary carbon centers in these compounds is very difficult. We developed stereoselective indium-mediated allylation to hydarzones bearing L-proline, which affords α,α-disubstituted α-amino acid derivatives with controlled quaternary carbon stereogenic centers.

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Residue requirement for 11/9 helical propensity of α/β-peptide

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Unnatural peptide oligomers with a strong tendency to adopt specific and predictable conformations in solution have been the subject of extensive investigation in recent years. Also α/β-peptides can adopt helical secondary structures in solution. We reported α/β-peptides containing L-Ala and cis-ACHC form 11/9-helix. We study the effects of variations in different α-residue substitutions on the propensity of α/β-pentapeptides. The third α-residue is replaced with D-Ala, Aib, L-Val and Gly. These α-residue changes will effect on 11/9-helical propensity.We synthesize and crystallize those α/β-pentapeptides. We report the residue requirement for 11/9-helical propensity of α/β-pentapeptides.

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Direct water free synthesis of ionic liquids - *Dual roles of orthoester*

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부산대학교 화학과

Recently, room temperature ionic liquids(RTILs) have obtained great attentions due to their unique properties, for example, great solvating abilities, thermal and chemical stabilities, high conducting properties and reusabilities as a green solvent. Since Wilkes et al. published air and water stable low melting imidazolium salts, weakly coordinating anions such as BF_4^- , PF_6^- , $(CF_3SO_2)_2N^-$ are the most popular because they provide low melting points and high thermal stabilities. The traditional method requires multistep process involving alkyl halide salt formation, anion exchange, and removal of metal halides. So far, no direct synthetic route for the synthesis of both coordinating and non-coordinating anion RTILs has been developed yet. Herein, we would like to present one-pot water free synthetic method using orthoesters, which play a role of not only alkylating agent but also dehydrating agent.

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Benzothiadiazole cored donor materials for organic photovoltaic cells

전용준 홍종인*

서울대학교 화학부

Since the first report of organic solar cells (OSCs) by Tang, the development of OSCs has attracted considerable attention due to their advantages of easy synthesis, low cost and easy device fabrication. Generally, organic small molecules based on oligothiophene were used as donor materials for heterojunction solar cells due to good charge transport ability. A benzothiadiazole unit was used as low band gap donor materials due to their broad absorption spectra.To improve performance of heterojunction solar cells, we introduced new low bandgap donor materials, consisting of benzothiadiazole, naphthalene, benzothiophene and thiophene. Details of the synthesis, photophysical, electrochemical and theoretical studies and device data will be presented.

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Synthetic Chloride Transporters Triggered by Enzymes

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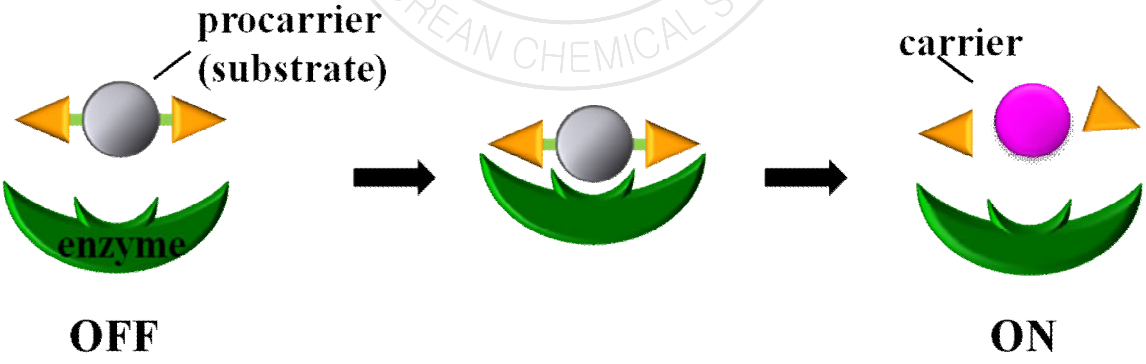
연세대학교 화학과

Chloride is an abundant anion in the biological system and is related to several diseases. We synthesized molecules that could bind and transport chloride across a lipid bilayer membrane upon addition of glycosidases. Procarriers contain glucosyl units that interfere not only the binding of chloride sterically but also its partitioning into the lipid membrane. The enzymatic removal of the glucosyl units in-situ generates an active transporter which can bind and transport chloride across a POPC (1-palmitoyl-2-oleoyl-sn-glycero-3-phosphocholine) membrane. Details will be described in the presentation.



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Radical addition to C=N bond of L-proline-derived hydrazones in aqueous media: Asymmetric synthesis of chiral amines

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Chiral amines have proven to be powerful pharmacophores for defining new pharmaceutical drugs. Despite the need for and continued interest in chiral amines, their synthesis remains challenging. Especially, studies of synthesis chiral amines in the present of water have been rarely reported. Using water as a solvent in organic reactions is strong desires of chemist, because of its eco-friendly and economical nature. We introduced L-proline to control the stereoselectivities and designed the radical addition reactions in aqueous media with two different radical initiator, indium and triethylborane. Treatment of L-proline-derived hydrazones with various alkyl iodides and two different radical initiators gave the corresponding chiral amines in high yields and good diastereomeric ratios.

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Ratiometric response for cadmium recognition pyrene labelled peptide sensor

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Pyrene labelled peptide is synthesized using a solid phase synthesis. This peptide sensor has selectivity for Cd(II) ions. This fluorescent sensors shows ratiometric response for only Cd(II) ions. Adding Cd(II) ions in the sensor, monomer is quenching and excimer appear in HEPES buffer (pH 7.4) containing aqueous solution. It shows same response in 100% organic solution. This sensor binds Cd(II) ions with 1:1 ratio.

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Colorimetric and fluorescent chemodosimeter for sensing of Hg(II) ions using amino acid cysteine with an ICT fluorophore in aqueous solution

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Recently, various colorimetric sensors were developed for detection of heavy metal ions. Most of them work in organic solution and have low selectivity. Using cysteine for receptor, the sensors have no selectivity for specific analyte. We synthesized highly sensitive and selective chemodosimeter based on cysteine with ICT fluorophore. This sensor has response for and Hg(II) ions in aqueous solution. When Hg(II) was added to this sensor, this showed turn-off of fluorescent response and red shift of colorimetric response. This sensor makes new bond with Hg(II) ions. Even if add metal chelation EDTA, the response didn’t return back to its former state. Reaction rate of chemodosimeter is commonly slow. However, reaction of this sensor based on Cysteine finished within 5 min.

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Selective and Sensitive chemosensor for Hg(II) ions based on Tryptophan amino acid and NBD derivative fluorophore with PET mechanism

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Chemosensor which has a NBD derivative labelled Tryptophan is synthesized in solid phase synthesis. NBD has used fluorophore which has long excitation wavelength for sensing metal ions with Internal charge transfer system (ICT) . We developed ABD which was derived from NBD. This developed fluorophore has dimethyl-amine group and sulfonamide group instead of nitro group and amine group. Tryptophan amino acid plays a role as quencher. The sensor shows sensitive and selective response to Hg(II) ions among various metal ions. When Hg(II) ions were added to this sensor, it shows Turn-on response.

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Sensitively Monitoring Arsenic in Aqueous Solution Based on Dansylated Peptide

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The detection and quantification of arsenic ions are important because its contamination of groundwater and toxic effects on humans have been a serious problem. As peptide is water-soluble and biologically compatible, chemosensor based on peptide is a promising route for monitoring arsenic ions in drinking water. A fluorescent chemosensor based on dansylated peptide showed selective and sensitive response to arsenic ions among various metal ions in aqueous solutions.

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Highly feasible selective fluorescent sensor for detection of heparin using AIE fluorophore in aqueous solution

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Heparin is a highly sulfated acidic linear polysaccharide. It plays important physiological role through the electrostatic interaction with proteins that are involve in the clotting process of blood. Heparin is used as an anticoagulant during surgeries, so it is important to monitor the heparin levels to avoid complications such as hemorrhage or thrombocytopenia induced by heparin overdose. The therapeutic dosing level of heparin is 2-8 U/mL (17-67 μM) during cardiovascular surgery and 0.2-1.2 U/mL (1.7-10 μM) in postoperative and long-term care. The development of quick and reliable methods that allow heparin detection and quantification is of practical importance. Till now we had many fluorescent chemosensors using the aggregation induced emission (AIE) property. We synthesized chemosensor based on the tripeptide with Tetraphenylethylene (TPE) as the AIE fluorophore. This sensor is pH independent and 100% water soluble owing to the presence of arginine (pKa=12.48) and lysine (pKa=10.79). AIE fluorophores show less fluorescence in the soluble form. This sensor shows large increase in fluorescence after analyte is added to the sensor with red shift. Even at High pH there is high fluorescence emission as expected because of the hydrogen bonding interaction of the heparin with the sensor making it feasible to use even at the pH beyond the pKa's of both the lysine and arginine residues.

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Hexaethylene Glycol Bridged Dicatioic Ionic Liquids: Significantly Enhanced Reactivity of KF in Nucleophilic Fluorination as Organic Promoter

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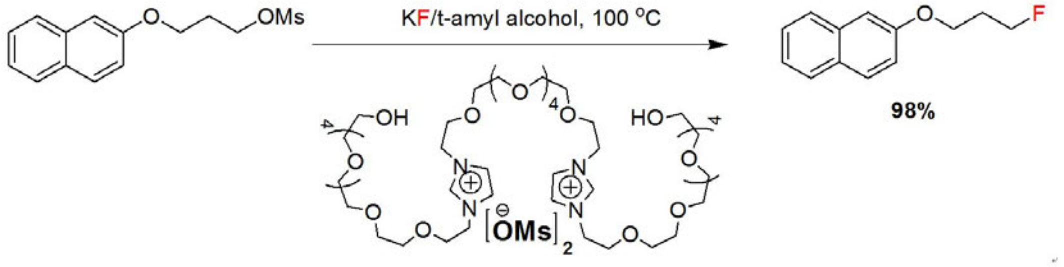
인하대학교 화학과

Imidazolium based ionic liquids (ILs) can act as a powerful media in various organic transformations as solvent and well as catalysts. We have designed and prepared well-tailored hexa-ethylene glycol bridged dicationic imidazolium based ionic liquids as multifunctional organic promoter for nucleophilic fluorinations using potassium fluoride (KF) as a salt in tert-amyl alcohol at 100 °C. These hexa-ethylene glycol bridged dicationic imidazolium based ionic liquids could enhance the reactivity of KF significantly in nucleophilic fluorinations. Furthermore, by their synergistic effect, the combination of hexa-ethylene glycol bridged dicationic imidazolium based ionic liquids and *tert*-amyl alcohol media system showed tremendous efficiency in the fluorination of base-sensitive substrates.



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발표종류: 포스터, 발표일시: 수 16:00~19:00

Boron subphthalocyanine Nanospheres with Enhanced Antibacterial Efficiency

RoyIndranil Raghunandan Hota[1] 백강균[2] 김기문[3,*]

포항공과대학교 Chemistry [1]포항공과대학교 지능초분자연구단 화학과 [2]기초과학연구원 복잡계자기조립연구단 [3]포항공과대학교 화학과

The emergence of antibiotic-resistance among pathogenic bacteria has lead efforts to find alternative antimicrobial therapeutics such as photodynamic therapy (PDT). The photodynamic inactivation of antibiotic-resistant bacteria has been explored only with limited success. However, multifunctional nanomaterials can be utilized not only for the killing of pathogenic and antibiotic-resistant bacteria, but also for targeting and labeling. Here, we demonstrate a facile fabrication of covalently bonded, multifunctional boron subphthalocyanine (BsubPc) nanospheres with a hollow interior, through thiol-ene click chemistry in solution without using any template, pre-organized structure, or emulsifier. The BsubPc nanospheres have been characterized by SEM, TEM and various spectroscopic methods. The size of the nanospheres can be tuned by regulating the composition of reaction medium, temperature and polymerization condition. Applications of the BsubPc nanospheres in target, label and photodynamic inactivation of antibiotic-resistant bacteria have been studied. Details of this work will be presented.

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Tandem Rh(III)-Catalyzed Alkenylation and Cyclization of *N*-Benzyltriflamides

박지혜* 한상일 신영미

성균관대학교 약학과

Isoindoline heterocycles have demonstrated potential in organic and medicinal chemistry as they exhibit diverse biological activities and interesting chemical properties. For example, the isoindoline motif is present in molecules that act as selective PPARδ agonists, molecular chaperone Hsp90 inhibitors, endothelin-A receptor antagonists, and dipeptidyl peptidases inhibitors. Moreover, isoindoline derivatives are very crucial constituents in the field of material science as attractive candidates for organic light-emitting devices. Therefore, the development of novel and highly efficient strategies for the formation of these heterocyclic architectures is an area of great interest in organic synthesis. Transition-metal-catalyzed C-H bond activation has emerged as an atom economical process to produce structurally diverse organic molecules due to the minimization of stoichiometric metallic waste. Thus, the cross-coupling reactions via C-H bond activation can lead to an improved overall efficiency of the desired transformation. Since the pioneering efforts of Fujiwara and Moritani, remarkable progress has been made on the oxidative olefination of arenes using alkenes under palladium catalysis to directly functionalize arene C-H bonds. In contrast to the vast majority of reports on the palladium-catalyzed olefinations, the oxidative C-H olefinations using rhodium catalysts, which often allow lower catalytic loadings, higher selectivities, and broad substrate scope, have been much less explored. For instance, Matsumoto and Yoshida described an oxidative coupling reaction between benzenes and ethylene using cyclometalated Rh(III) catalysts to afford styrenes. Notably, Satoh and Miura and Ackermann respectively reported Rh(III)- and Ru(II)-catalyzed oxidative coupling and intramolecular cyclization between benzoic acids and acrylates. Li disclosed Rh(III)-catalyzed tandem oxidative olefination and aza-Michael reaction of secondary benzamides with *α,β*-unsaturated alkenes. In addition, a great deal of effort has been devoted to the selective olefination of arenes with various directing groups such as pyridinyl, hydroxyl, esters, anilides, carbamates, and ketones/amides. A triflamide moiety as a directing group was first introduced by Yu for the palladium-catalyzed C-H bond functionalization, and can be transformed to a range of synthetically useful functional groups. Our continued efforts in rhodium- or palladium-catalyzed C-H bond activation and oxidative acylation reactions prompted us to explore the coupling reaction of *N*-benzyltriflamides with olefins. In conclusion, we developed the facile and efficient strategy for the construction of isoindolines via rhodium(III)-catalyzed oxidative ortho-alkenylation of *N*-benzyltriflamides with olefins followed by intramolecular cyclization via sp^2 C-H bond activation. Further applications to the synthesis of biologically active compounds and the expansion of the scope to unactivated sp^3 C-H bonds are in progress.

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Synthesis of chiral 6-membered N-heterocyclic carbene palladium complexes and their application to intramolecular α-arylation of amides

오경환 박진균*

부산대학교 화학과

N-Heterocyclic carbene ligands (NHCs) have unique properties compared to phosphine ligands in terms of their strong σ-donating abilities and large cone angles. Recently, various 5-membered NHCs have been developed for the organocatalysis and transition metal catalysis. Especially in palladium catalyzed reaction, chiral 5-NHC palladium complexes have been successfully designed and utilized, however, few chiral 6-NHC Pd complexes are known. Herein, we will present the synthesis of chiral annulated 6-NHC Pd complexes identified by NMR and X-ray analysis. Because the chiral annulated 6-NHC precursor has additional binding site, we could synthesize mono and bi Pd complex, respectively. We also successfully synthesized bimetallic complex which has Pd on NHC and Rh on imidazoline ring. Initially, we decided to test 6-NHC palladium complex in intramolecular α-arylation comparing with the known 5-NHC palladium complexes. Despite of low selectivities in preliminary results, we are still focusing on changing the substituents of 6-NHC to improve enantioselectivity.

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Cu-Catalyzed Direct Esterification of 2-Carbonyl Substituted Phenols with Acyl Equivalents

박지혜 김인수[1,*]

성균관대학교 약학과 [1]성균관대학교 약학대학/약학과

Esterification is one of the vital chemical reactions that have been extensively used in the chemical and pharmaceutical industries. The general strategies usually involve the activation of the carboxylic acid as an acyl halide, anhydride, or activated ester followed by nucleophilic substitution with alcohols. Although various research groups have exploited and developed several methods to the formation of esters, oxidative esterification has received increasing attention from the atom economic point of view, and has become an economical alternative to traditional ester formation. Recent efforts have been made towards the oxidative coupling between aldehydes and alcohols. A variety of conditions have been executed such as those using a stoichiometric oxidant, *N*-heterocyclic carbene activation, and transition metal-mediated processes.An attractive alternative is the direct formation of esters from the alcohol oxidation level, which represent a step forward toward green, economic, and sustainable processes. Alcohols are available at low cost in great structural diversity, and are easy to handle and to store. Also, alcohols can be readily oxidized into aldehydes under metal catalysis. Scheidt described a tandem oxidation of allylic and benzylic alcohols to esters using *N*-heterocyclic carbenes as catalysts, which required large amounts of MnO_2 as the oxidant. Traditional methods for synthesizing these compounds include esterification of phenols, trans-esterifications and Baeyer-Villiger oxidation reactions. These reactions were often required strong acidic or basic conditions, which limit the scope of functional groups. Recently, Chen and Pan described palladium/NHC and ruthenium/NHC-catalayzed oxidative esterification of phenols with benzylic alcohols to afford aryl benzoate derivatives. However there is no report for the oxidative esterification of 2-carbonyl substituted phenols from the alcohol oxidation level. In particular, 2-carbonyl substituted aryl and alkylbenzoates are found to be important precursor for biologically active moieties such as flavanols and benzopyrans.

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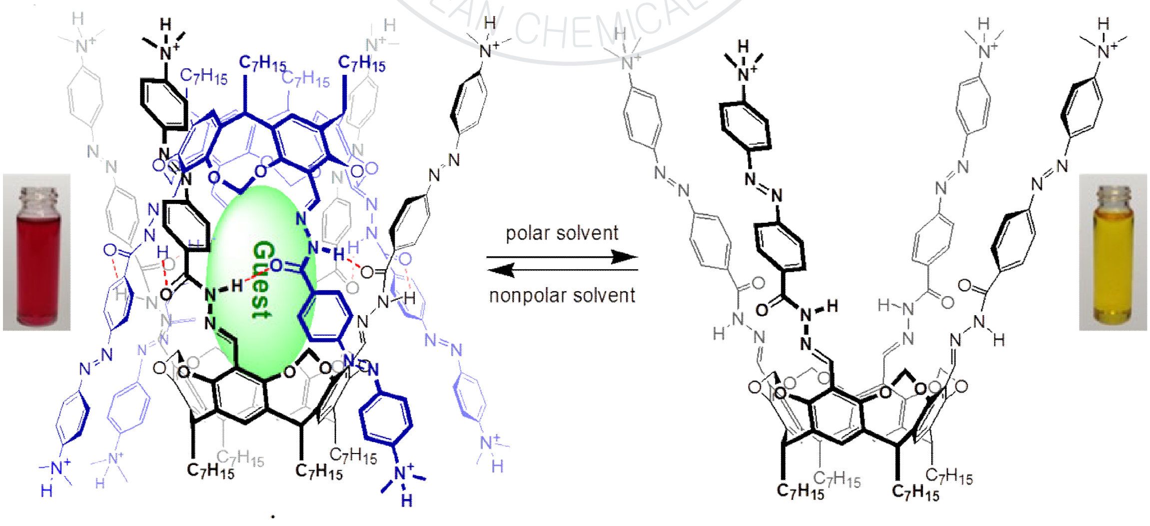
Naked-eye detection of the formation of a self-assembled molecular capsule

김조원 박연실 백경수*

숭실대학교 화학과

A new chromogenic self-assembled molecular capsule **G@1**$_2$ was developed by the introduction of four azobenzene moieties on the upper rim of a resorcin[4]arene-based amidoimino-cavitand. Cavitand **1** self-assembled to molecular capsules **G@1**$_2$ in the presence of suitable guests via the eight intermolecular N-H···O=C hydrogen bonds, and capsular complex **G@1**$_2$ showed a large bathochromic shift upon the addition of organic acid, which allowed the naked-eye detection of its formation from the color change of yellow to red according to the interconversion of cavitand to dimeric capsule.



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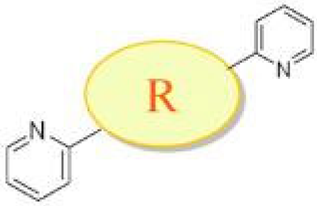
Electron transport materials based on heterocycle which has nitrogen-rich ring for OLEDs

이다현 노영리 윤순병 SHAIK BAJI 장용주 이상경*

경상대학교 화학과

The high electron mobility compounds can be used for electron transport layer in OLEDs. So novel nitrogen-rich heterocycle compound was designed and synthesized. The compound was synthesized by Suzuki coupling reaction. The obtained compound was confirmed by 1H-NMR and 13C-NMR. The compound was exhibited good thermal stability. Details of synthesis, characterization, thermal, and electrochemical properties of synthesized novel material will be presented.



R = Nitrogen rich heterocyclic molecules

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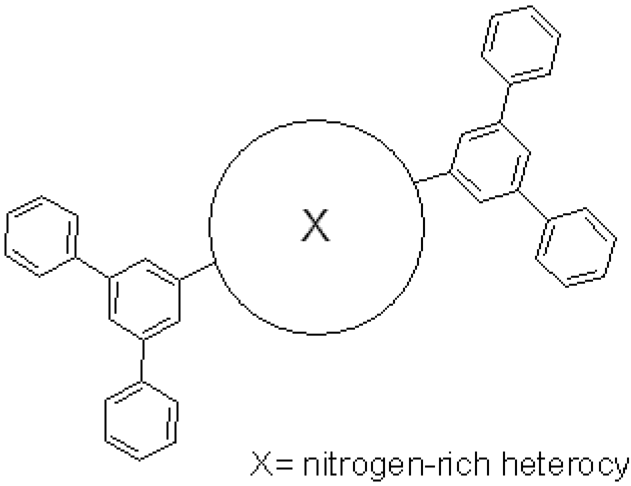
Synthesis and Characterization of Novel Material for Electron Transfer Layer in Organic Light Emitting Diodes (OLEDs)

노영리 윤순병 SHAIK BAJI 이다현 장용주 이상경*

경상대학교 화학과

Nitrogen-rich heterocyclic molecules have focusing for development of electron transporting materials (ETMs) because they have high electron mobility. The heterocycle compound which has nitrogen-rich was designed and synthesized for Electron Transport Material (ETM). The obtained material was characterized by 1H-NMR and 13C-NMR. It's optical, thermal and electrochemical properties were measured by UV absorption, photoluminescence (PL), thermal gravimetric analysis (TGA), differential scanning calorimetry (DSC) and cyclic voltammetry (CV). As a result, novel compound was exhibited high Td of 285 oC, high Tg of 123 oC. The absorption maximum spectra of the materials were measured at 257,292 nm . The PL maximum spectra of the materials were observed at about 457 nm. Herein reported for the development of synthetic method, special optical character, and electrochemical properties of the synthesized novel material.



X= nitrogen-rich heterocycle

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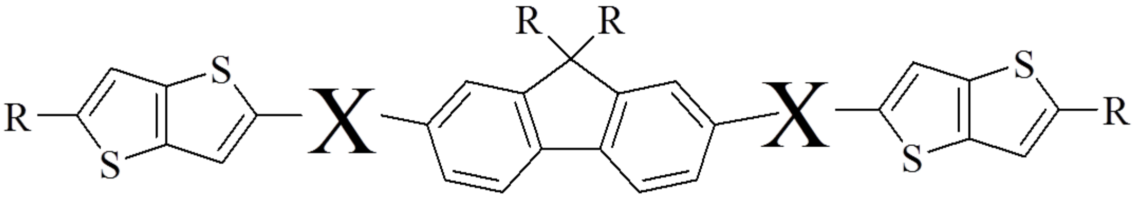
Synthesis and TFT Properties of Novel Conjugated Compound for Organic Thin Film Transistors

윤순병 노영리 SHAIK BAJI 장용주 이다현 이상경[*]

경상대학교 화학과

Synthesis and physical properties of a novel p-type organic thin film transistors (OTFTs) materials containing thiophene, benzene, thieno[3,2-b]thiophene and fluorene derivatives were studied. Suzuki and Stille coupling reaction were applicated for the synthesis of these materials at the final step. The obtained compound was confirmed by ESI-Mass, FT-IR, 1H-NMR, 13C-NMR spectroscopy and elemental analysis. The synthesized FCTT and FCBT have moderate solubility in common organic solvents such as chloroform, methylene chloride and THF. The date of thermal gravimetric analysis (TGA) differential scanning calorimetry(DSC), optical and electrochemical properties of the novel synthesized FCTT and FCBT will be presented.



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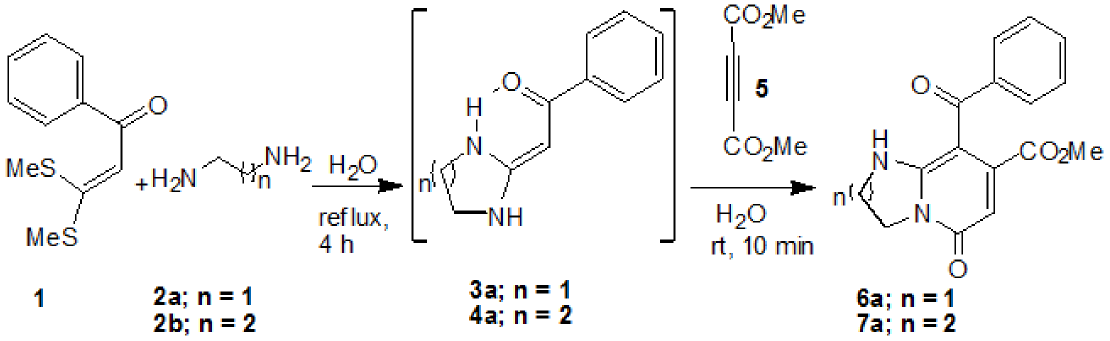
Synthesis of Imidazo[1,2-a]pyridines and Pyrido[1,2-a]pyrimidines in Water and their SNAr Cyclizations

장용주 윤순병 노영리 SHAIK BAJI 이다현 이상경*

경상대학교 화학과

Synthesis of terahydroimidazo[1,2-α]pyridines and tetrahydropyrido[1,2-α] pyrimidines by a one-pot and three component reaction of α-oxoketenedithioacetals, diamines and DMAD in water has been described. Different routes for accessing the disired compounds were examined and a few specially designed-substrates have been utilized further to afford the new imidazo and pyrido fused [1,8] naphthyridine tetracyclic compound by SNAr intramolecular cyclization.



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Pd-Catalyzed Oxidative Coupling of Arene C?H Bonds with Benzylic Ethers

한상일* 박지혜 신영미

성균관대학교 약학과

Transition metal-catalyzed selective cross-coupling reaction via C?H bond activation has emerged as an attractive alternative to traditional cross-coupling reactions due to the minimization of stoichiometric metallic waste and the costs associated with the preparation of starting materials. Thus, cross-coupling reactions via C?H bond activation can lead to an improved overall efficiency of the desired transformation. Since the pioneering efforts of Murai, remarkable progress has been made on carbon-carbon cross-coupling reactions via C?H bond activation. In particular, most of C?H bond activation process generally rely on the strategies of directing group assisted C?H bond functionalization and cross dehydrogenative coupling (CDC). Recently, transition metal-catalyzed oxidative *ortho*-acylation between arene C?H bonds bearing conventional directing groups and aldehydes or alcohols as acyl sources have been described. Catalytic decarboxylative acylations of aromatic C?H bonds using α-oxocarboxylic acids as acyl surrogates were also reported. Recently, a palladium-catalyzed acylation of inactive sp^2 C?H bonds via C?H, C?C, and C?O bond cleavage of toluenes. diketones, and carboxylic acids was respectively reported. In addition, Yang and Wu demonstrated a palladium-catalyzed direct C?H acylation using arylmethyl amines as new acylation reagents.Benzylic ethers constitute one of the common protecting groups for alcohols. The C?O bond of benzylic ethers is readily cleaved under a variety of either oxidative or reductive conditions. In particular, oxidative reactions of methylene carbons in benzyl ethers are important transformations because they can convert chemically stable moieties into reactive functional groups, including aldehydes, esters, and carboxylic acids, that are widely used in organic synthesis. Since a first report on the formation of benzaldehydes from benzyl methyl ethers by Markees in 1958, a number of methods for the formation of benzaldehydes via the oxidative cleavage of benzylic C?O bonds have been described under various conditions, such as NBS/H_2O, TEMPO, HNO_3,

$Cu(NO_3)_2$, and DDQ. However, it is no report concerning the behavior of benzylic ethers when treated with *tert*-butyl hydroperoxide (TBHP) as a mild oxidant. As part of an ongoing research program directed toward the development of catalytic acylation reactions of inactive C?H bonds, we became interested in developing oxidative acylation reactions using benzylic ethers. Herein, we present the palladium-catalyzed *ortho*-acylation of arenes C?H bonds with benzylic ethers under *tert*-butyl hydroperoxide (TBHP) to afford aryl ketones.

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Planar Conjugated Organic Thin Film Transistors Compounds; Synthesis and Characterization

SHAIK BAJI 윤순병 노영리 장용주 이다현 이상경*

경상대학교 화학과

Organic semiconductors provide many advantages over the inorganic semiconductors such as design of molecular structures for mobility optimization, high ?exibility, low cost of materials fabrication, ease for large area processing and compatibility with ?exible substrates. Thus thin film transistors made of organic semiconductors have several applications in active matrix display, RIF tags and smart cards etc. One of the important requirements of organic semiconductor for exhibiting good mobility is planar structure. The planar compound pentacene has exhibited good mobility, but the insolubility property hindered its practical application. Based on this property, thienothiophene and fluorene based planar compounds designed. For solubility purpose alkyl chains were introduced. The optical, thermal and electrochemical properties of the compounds were determined. The compounds have shown good thermal and electrochemical stability. Based on these results, we can expect OTFTs prepared by using these materials can be exhibit high mobility.

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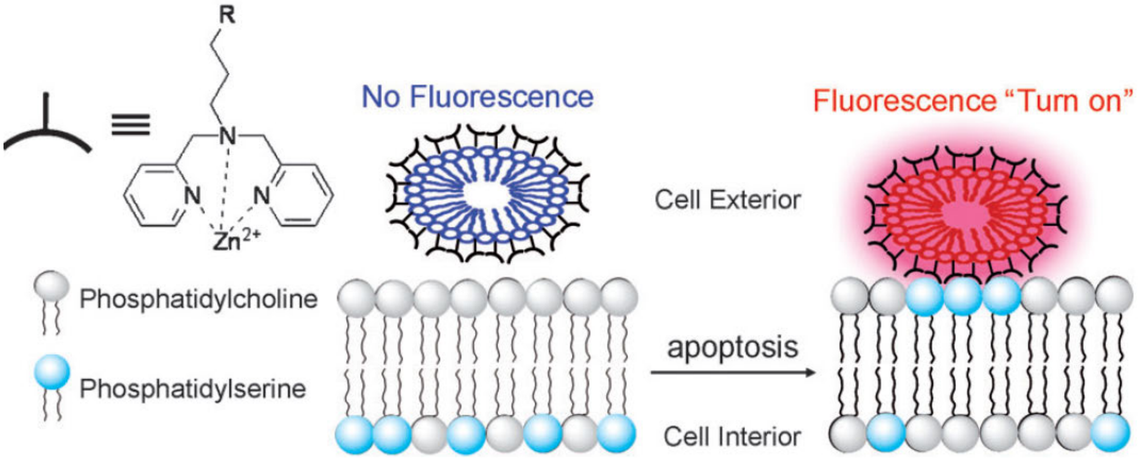
Turn-On Fluorescence Detection of Apoptotic Cells Using a Zinc(II)-Dipicolylamine-Functionalized Poly(diacetylene) Liposome

마동희 안교한*

포항공과대학교 화학과

Apoptosis, the process of programmed cell death, is essential for embryonic development, function of the immune system, and the maintenance of tissue homeostasis.[1] Dysregulation of apoptosis has been implicated in various pathological conditions, such as neurodegenerative and autoimmune diseases.[2] In healthy cells, phosphatidylcholine (PC) and sphingomyelin (SM) are exposed on the extracellular surface of the plasma membrane, whereas phosphatidylserine (PS) and phosphatidylethanolamine (PE) are located on the cytosolic surface. When cells undergo apoptosis, redistribution of the phospholipids occurs that involves the translocation of PS to the outer layer of the membrane.[3] Recently, Zn.$^{\text{II.}}$ complexes of bis(pyridin-2-ylmethyl)amine (DPA) received attention as artificial PS recognition motifs, thus replacing Annexin V in the development of detection systems for apoptotic cells. We have developed a liposome-based fluorescence sensing system for apoptotic cells from stimuli-responsive poly(diacetylene)-liposomes for the first time. Liposome 2 selectively senses vesicles of PS over other vesicles such as those of PC, SM, and PE, thereby showing a spectral change from blue to reddish purple. This liposome-based sensing system also responds to apoptotic cells in the fluorescence turn-on mode. As a result, liposome 2 can be used to sense apoptotic cells, as demonstrated by confocal fluorescence microscopy as well by FACS analysis. The turn-on response of the present system eliminates the washing steps required for most dye-conjugated sensing systems.Reference[1] C. B. Thompson, Science 1995, 267, 1456.[2] H. Okada, T. W. Mak, Nat. Rev. Cancer 2004, 4, 592.[3] P. A. Leventis, S. Grinstein, Annu. Rev. Biophys. 2010, 39, 407.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N
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Zn2+
No Fluorescence
Fluorescence "Turn on"
Cell Exterior
Phosphatidylcholine
Phosphatidylserine
apoptosis
Cell Interior

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Gold-state elevation approach to suppress side reactions in gold sensing systems based on alkyne activation

전용웅 안교한*

포항공과대학교 화학과

Gold complexes have been intensively used in various research fields for their unique chemical and biological properties. As a result of cytotoxicity to DNA and enzymes, for instance, gold complexes have been investigated as anticancer and antirheumatoid agents.(1) Therefore, efficient detection systems for the gold species are demanded.Although many reported probes for gold ions show high selectivity toward gold ions with turn-on fluorescence response, they provide side reactions in the gold ion-promoted chemical conversion which can complicate the quantification, as we raised this issue earlier.(2) Also, the non-signaling processes lower the probe's sensitivity toward gold ions.We have found the novel approach alleviates the side reactions and also improves the slow response rate and low sensitivity of the previous probes. Furthermore, from the new sensing system we can readily construct its fluorescence resonance energy transfer (FRET) system, which allows analyte quantification with minimized interference from the environmental parameters.(3) ref:(1). (a) Finkelstein, A.; Walz, D.; Batista, V.; Mizraji, M.; Roisman, F.; Misher, A. Ann. Rheum. Dis. 1976, 35, 2517. (b) Tomioka, R.; King Jr, T. E. Am. J. Respir. Crit. Care Med. 1997, 155, 1011. (c) Shaw, C. F. Chem. Rev. 1999, 99, 2589. (2). Seo, H.; Jun, M. E.; Egorova, O. A.; Lee, K.-H.; Kim, K.-T.; Ahn, K. H. Org. Lett. 2012, 14, 5062(3). (a) Fan, J.; Hu, M.; Zhan, P.; Peng, X. Chem. Soc. Rev. 2013, 42, 29. (b) Yuan, L.; Lin, W.; Zheng, K.; Zhu, S. Acc. Chem. Res. 2013, 46, 1462.

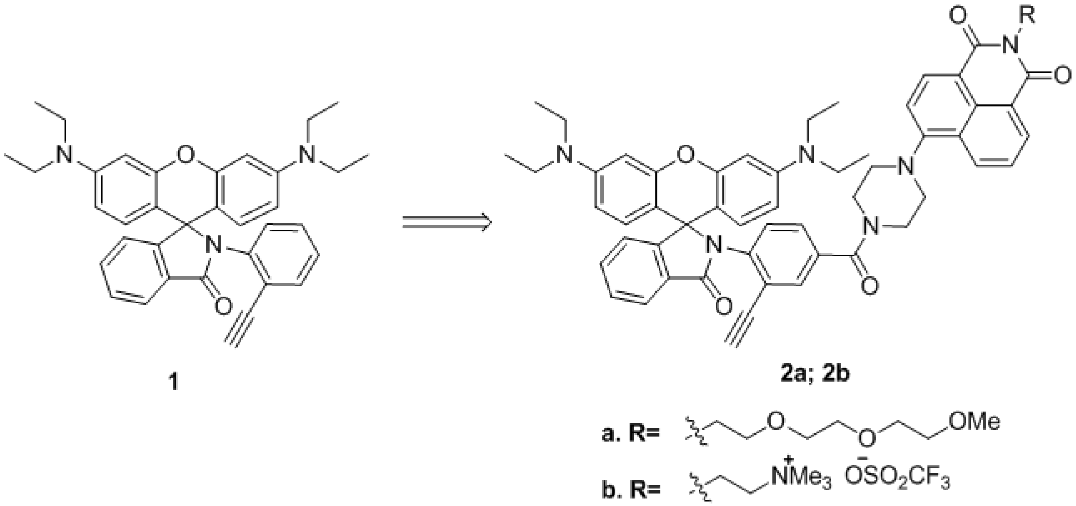

Figure 1. A new probe 1 and its FRET versions 5a and 5b.

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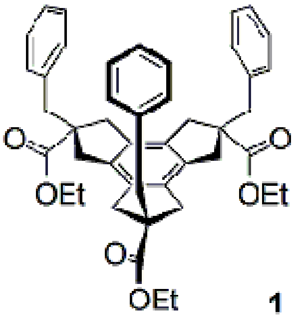
C_{3V}-Symmetric Tripodal Fluorescent Anion Molecular Sensorsbased on *cis,cis,cis*-2,5,8-tribenzyltrindane-2,5,8-tricarboxylate

김원 최홍진*

경북대학교 응용화학과

Novel C_{3v}-symmetric tripodal anion receptors having guanidine recognition motif with 2-aminobenzimidazole (2) and urea recognition motif with coumarin fluorephore (3) were synthesized from *cis,cis,cis*-2,5,8-tribenzyltrindane-2,5,8-tricarboxylate (1). The C_{3v}-symmetric scaffold 1 has non-polar benzyl moieties on one side and polar ester moieties on the other side. These moieties were selectively functionalized to afford the C_{3v}-symmetric anion molecular sensors to recognize selectively and effectively towards anions with C_{3v}-symmetry guests such as F^-, Cl^-, Br^-, I^-, $H_2PO_4^-$, HSO_4^-, NO_3^-, HCO_3^- ions, expecting shape-selectivity.Interestingly the tripodal receptor 2 showed a superior recognition towards $H_2PO_4^-$ by NMR titration, but selectively recognized with HSO_4^- emitting blue fluorescence under UV irradiation, which can be further developed to fluorescent anion sensors. Anion recognition of tripodal urea receptor 3 with coumarin fluorephore also will be presented as potentional fluorescent anion sensor.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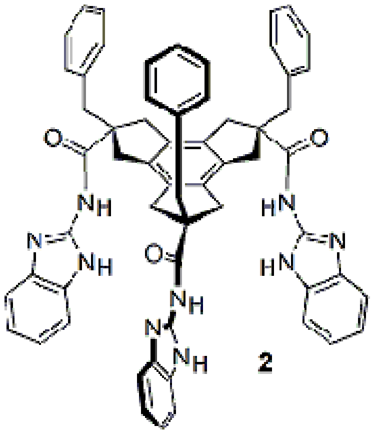
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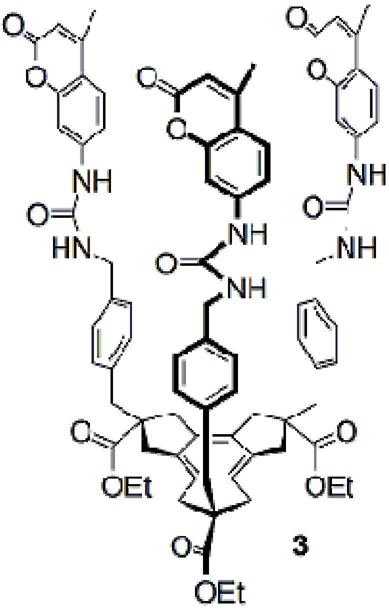
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1-Sulfonyl-1,2,3-triazoles: Conventional Precursors for Rh carbenoides

이동진 신진환 유은정*

강원대학교 화학과

Because the stability of the 1,2,3,-triazole is affected by the substituents at the N1, C4, and C5 atoms of the cycle, triazoles bearing a sulfonyl group at the N1 atom exist in equilibrium with diazoimine tautomer. Recently, many research group took advantage of this process by trapping diazoimine with a Rh(II) catalyst to produce the Rh(II) azavinyl carbenes. This intermediate possessed reactivity inherent for Rh(II) carbenoids such as addition to carbon-carbon multiple bonds and insertion into C-H bonds. Undoubtedly, development of new method to access Rh(II) carbene species from readily available 1-sulfonyl-1,2,3,triazoles could expand the scope of carbene chemistry.

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Facile synthesis of natural moracin compounds using $Pd(OAc)_2$/ $P(^tBu)_3$-HBF_4 as a Sonogashira coupling reagent

윤소라 전종갑*

한림대학교 화학과

An efficient and practical synthesis of natural moracins, which have diverse range of biological properties including anticancer, antioxidant, and antibacterial activities, has been achieved using $Pd(OAc)_2$/ $P(^tBu)_3$-HBF_4 as a Sonogashira coupling reagent which solved the unreactive problems in case of higher electron density of haloaryl compounds in the reaction. The lowered electron density of haloaryl compounds with acetylation and the use of modified Sonogashira coupling reagent from $PdCl_2(PPh_3)_2$ to $Pd(OAc)_2$/ $P(^tBu)_3$-HBF_4smoothly produce the benzofuran structures in the syntheses of moracins M, N and S. Electron deficient haloaryl compound containing aldehyde, however, is easily form the benzofuran using original Sonogashira condition, and utilized for the first synthesis of moracin Y.

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Synthetic approach towards new bioactive piperidine alkaloids

KONGARADAMODAR 문인수[1] 전종갑[1,*]

한림대학교 응용화학연구소 [1]한림대학교 화학과

Nitrogen containing compounds are very widely distributed in nature and are essential to life. They play a vital role in the metabolism of all living cells. At present, greater than 75% drugs and drug candidates incorporate amine functionality.1 Among the numerous naturally occurring nitrogen containing compounds, piperidine skeleton is an important structural feature found in various secondary metabolites and biologically active compounds.2 In particular, simple 2-alkyl-piperidines3 [e.g.; coniine 1 and pipecolic acid 2] have become important targets for the synthesis over the past few decades due to their scarcity in natural sources, wide array of structural diversity and notable physiological effects. Herein, we wish to present the synthetic approach towards new bioactive piperidines of this class using N-tert-butanesulfinyl imines which can be prepared from readily available chiral N-tert-butanesulfinamide and aldehyde (or ketone), exhibit unique reactivity, hydrolytic stability and stereoselectivity in various reactions have been proven to be extremely versatile chiral reagents.4*References:*1. MDL. MDL Drug Data Report. MDL Information System Inc. San Leandro CA; G. Liu, O. A. Cogan, J. A. Ellman. J. Am. Chem. Soc. 1997, 119, 9913.2. (a) Strunz, G. M.; Findlay, J. A. In The Alkaloids; Brossi, A., Ed.; Academic Press: San Diego, 1986; Vol. 26, p 89; (b) Fodor, G. B.; Colasanti, B. In Alkaloids: Chemical and Biological Properties; Pelletier, S. W., Ed.; Wiley: New York, 1986; Vol. 3, p 1. 3. For reviews on piperidine alkaloids, see: (a) Plunkett, A. O. Nat. Prod. Rep. 1994, 11, 581. (b) Hammann, P. In Organic Synthesis Highlights II; Waldmann, H., Ed.; VCH: Weinheim; 1995; pp 323. (c) Schneider, M. J. In Alkaloids: Chemical and Biological Perspectives; Pelletier, S. W., Ed.; Wiley: New York, 1996; Vol. 10, pp 155. (d) O’Hagan, D. Nat. Prod. Rep. 2000, 17, 435. (e) Bailey, P. D.; Millwood, P. A.; Smith, P. D. Chem. Comm. 1998, 633. 4. Robak, M. T.; Herbage, M. A., Ellman, J. A. Chem. Rev. 2010, 110, 3600.

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Synthesis of natural product piperlongumine and its derivatives

서영화 김철기 전종갑*

한림대학교 화학과

We wish to describe a convenient and general method for the synthesis of anticancer natural product Piperlongumine. This compound was extracted from the fruit of black pepper in Southern India and South-East Asia. It has been known that Piperlongumine showed better anticancer activity than taxol. Coupling reaction between Cinnamic acid and δ-valerolactam was utilized for the Piperlongumine synthesis. Derivatives of piperlongumine has been synthesized through similar methodology.

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Synthesis of biologically active benzo[*b*]furan natural compounds and their derivatives

유현호 전종갑*

한림대학교 화학과

We wish to describe an effective synthesis of benzo[*b*]furan natural compound Puerariafuran. This compound has been extracted from *Pueraria lobata Ohwil*. This is also known as nontoxic, and good for treating and preventing diabetic complications. Another benzo[*b*]furan natural compound Obovaten, which is isolated from the *persea obovatifolia* and known to have anticancer activity, has been synthesized from the Al_2O_3 mediated coupling reaction between phenol and α-brominated ketone compounds. And we will measure the effectiveness of derivatives.

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Facile Synthesis of Licochalcone C

김철기 전종갑*

한림대학교 화학과

Several chalcone compounds have been extracted and characterized from Licorice, perennial herb which grows in southern Europe, China, Russia and Turkey. Among these chalcone compounds, licochalcone C have been extracted from Licorice in china, and known to have several promising biological activities (antimutagenic, antiparasitic, antileishmanial, anti-ulcer, anti-oxidative and anti-inflammatory effects). Biological activities of licohalcone C have been known such as antioxidant and inhibitor of PTP1B enzyme, but not been fully elucidated. Licochalcone C was synthesized from commercially available 2,4-dihydroxybenzaldehde by using regioselective Al_2O_3-mediated C-prenylation followed by conventional Claisen-Schmidt condensation in basic condition. Direct water-accelerated [3,3]-sigmatropic rearrangement reaction of chalcones could not be employed in the licochalcone C synthesis due to the decomposition problems, however we found the regioselective C-prenylation using Al_2O_3 for a new additional licochalcone C synthesis.

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Synthesis of piceatannol derivatives

문인수 전종갑*

한림대학교 화학과

Stilbene is one of the polyphenolic compounds and exists as cis or trans isomer. Stilbene derivatives have exceptional antioxidant. The antioxidant activity of stilbene derivatives differs from the type of positions, substituents, and the structural isomers. Stilbene derivatives were synthesized according to the HATU reaction, Wittig-Horner reaction and Sonogashira coupling method.

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A Ratiometric Two-Photon Probe for Real-Time Imaging of Lysosomal pH

김형중 허철호 김환명*

아주대학교 에너지시스템학부

Acidic pH plays crucial roles in many aspects of cell metabolism. To extend our understanding of the roles of acidic environments in biology and pathology, it is essential to monitor subcellular pH values at the cell, tissue, and organism level. However, most conventional probes have limitations imposed by fluorescent turn-on responses at single detection window and/or their short excitation wavelength encountered. An attractive approach to the detection of pH value in live cells and tissues is ratiometric imaging with two-photon microscopy (TPM). TPM, which employs two near-infrared photons as the excitation source, offers a number of advantages including greater penetration depth (> 500 μm), localization of excitation, and longer observation times. We report small molecule and ratiometric TP probes (BH1-3 and BH1L) derived from benzimidazole for monitoring acidic pH in subcellular compartments. These probes have a bright two-photon excited fluorescence, a marked blue-to-green emission color change in response to pH 7.5-4.0 with pKa values of 4.9-6.1, a distinctive isoemissive point, negligible cytotoxicity, and high photostability, thereby allowing real-time quantitative imaging of intracellular pH.

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A proline-derived two-photon fluorescent probe for intracellular sodium ions

Sarkar Avik Ranjan <u>이효원</u>[1] 김환명[1,*]

아주대학교 나노정보융합기술연구소 [1]아주대학교 에너지시스템학부

The design of a synthetic probe to sense sodium ions is of extreme importance in the biomedical field because it plays vital roles in many physiological and pathological processes. In the detection of Na^+, a handful one-photon (OP) fluorescent probes have been reported in literatures. The main drawback of these probes is that they are bulky and suffer from difficulties in loading into live cells. The second one is their short excitation wavelength ($^+$ in biological processes is the use of two-photon microscopy (TPM), which utilizes two near-infrared photons of lower energy for the excitation. Previously, we reported Na^+ ion selective TP probe (ANa1) that has been selectively detect Na^+ in live cell and tissue by TPM. Based on promising properties of ANa1, herein, we report an efficient turn on TP probe (ANa2) that shows a maximum TP action cross-section of 80 GM with a dissociation constant (K_d^{TP}) value of 22 mM and strong TPEF enhancement in response to Na^+. This probe can selectively detect intracellular free Na^+ in live cells and living tissues without interference from other metal ions.

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Synthesis and Characterizations of the Copolymers with Indenoindene and Benzimidazole Moieties for Organic Solar Cells

백지연 서홍석[1,*]

부산대학교 자연과학대학/화학과 [1]부산대학교 화학과

The novel electron deficient moiety, dimethyl-2H-benzimidazole (MBI), and dihydroindeno[2,1-a]indene (ININE) unit as electron-rich group were incorporated by polymerization to generate the conjugated polymers including donor?acceptor pair for the organic polymer solar cell. ININE, MBI, and thiophene (or bithiophene) units were coupled by the reactions of Stille and Suzuki polymerization to produce poly(2,7-(5,5,10,10-tetrakis(2-ethylhexyl)-5,10-dihydroindeno[2,1-a]indene)-alt-5,5-(4′,7′-di-2-thienyl-2,2-dimethyl-2H-benzimidazole)) (PININEDTMBIs) (or PININEBBTMBIs). In structure of MBI, the sulfur atom at 2-position of 2,1,3-benzothiadiazole (BT) unit was substitute with dialkyl-substituted carbon, while keeping the 1,2-quinoid structure, to enhance the solubility of the polymers. The hole mobility (FETs) of PININEBBTMBI was 3.2 x 10-4 cm2/Vs which was more enhanced than that of PININEDTMBI (2.7 x 10-5 cm2/Vs) due to the introduction of bithiophene units. The device with the configuration of indium tin oxide (ITO)/poly(3,4-ethylenedioxythiophene) (PEDOT):polystyrene sulfonate (PSS)/polymer:PC71BM(1:4 w/w)/Al, annealed at 100 ℃ for 10 min showed a open circuit voltage of 0.78 V, a short-circuit current density of 6.66 mA/cm2, and a fill factor (FF) of 0.41, giving the PCE of 2.11%, under the condition of white-light illumination (AM 1.5 G, 100 mW/cm2).

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A Ratiometric Two-Photon Fluorescent Probe for Quantitative Imaging of Mitochondrial H_2S

허철호 김환명*

아주대학교 에너지시스템학부

Hydrogen sulfide (H_2S) is a multifunctional signaling molecule that exerts neuroprotective effects in oxidative stress. In mitochondria, endogenous production of H_2S has been recognized to exert protective effects in oxidative stress leading to the dysfunction and cell death. Herein, we report a mitochondria targeted two-photon probe, SHS-M2, that can be excited by 750 nm femtosecond pulses and employed for ratiometric detection of H_2S in live astrocytes and living brain slices using two-photon microscopy (TPM). SHS-M2 shows bright two-photon-excited fluorescence and a marked change in emission color from blue to yellow in response to H_2S, low cytotoxicity, easy loading, and minimum interference from other biologically relevant species including reactive sulfur, oxygen, and nitrogen species, thereby allowing quantitative analysis of H_2S levels. Molecular TPM imaging with SHS-M2 in astrocytes revealed that there is a correlation between the ratiometric analysis and expression levels of cystathionine β-synthase (CBS), the major enzyme that catalyzes H_2S production. In studies involving DJ-1, a Parkinson's disease (PD) gene, attenuated H_2S production in comparison with wild-type controls was observed in DJ-1-knockout astrocytes and brain slices, where CBS expression was decreased. These findings demonstrate that reduced H_2S levels in astrocytes may contribute to the development of PD and that SHS-M2 may be useful as a marker to detect a risk of neurodegenerative diseases, including PD.

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Synthesis and Properties of Conjugated Polymers Based on Tetrafluorophenylene for Organic Photovoltaics

백지연 서홍석[1,*]

부산대학교 자연과학대학/화학과 [1]부산대학교 화학과

Recently it appears that fluorinated polymer also demonstrates a noticeably improved short circuit current (Jsc) and/or fill factor (FF) in BHJ devices as opposed to those of the nonfluorinated analogue polymer-based devices. To study more this effect, we introduced 1,4-dibromotetra-fluorobenzene units ,which is the new strong electron withdrawing unit, adjacent to the donor moiety. We synthesized the new conjugated polymers; HS-5477, HS-5478, HS-5479, HS-5480, HS-5486, HS-5487, HS-5488 and HS-5489 which were synthesized by Suzuki coupling reaction and Stille polymerization. The UV-vis absorption onset of HS-5477, HS-5478, HS-5479 and HS-5480 were around 700 nm and their optical band gaps were about 1.60 eV. The range of the UV edges of HS-5486, HS-5487, HS-5488 and HS-5489 was from 760 to 890 nm and their optical band gaps were about 1.2 eV. The HOMO energy levels of four polymers based on carbazole unit (HS-5477, HS-5478, HS-5479 and HS-5480) were at 5.5 eV, their LUMO energy levels were at -3.8 eV, corresponding to the electrochemical band gap of around 1.6 eV. And the other four polymers based on benzodithiophene unit (HS-5486, HS-5487, HS-5488 and HS-5489) showed -5.5 ~ -5.7 eV of HOMO energy levels and their LUMO energy levels were at -4.2 ~ -4.4 eV, giving the electrochemical band gap of around 1.2 eV. Among the polymers, HS-5480 exhibited the greatest performance with Voc of 0.71 V, Jsc of 8.68 mA/cm2 and FF of 0.44, giving the power conversion efficiency of 2.71%.

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one-pot oxidative esterification of aldehyde using UHP and MsCl

김원미 이종찬[*]

중앙대학교 화학과

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oxidation of benzyl alcohol to benzaldehyde using UHP, MsCl

김성태 이종찬*

중앙대학교 화학과

oxidation of benzyl alcohol to benzaldehyde using UHP, MsCl

일시: 2014년 4월 16~18일(수~금) 3일간
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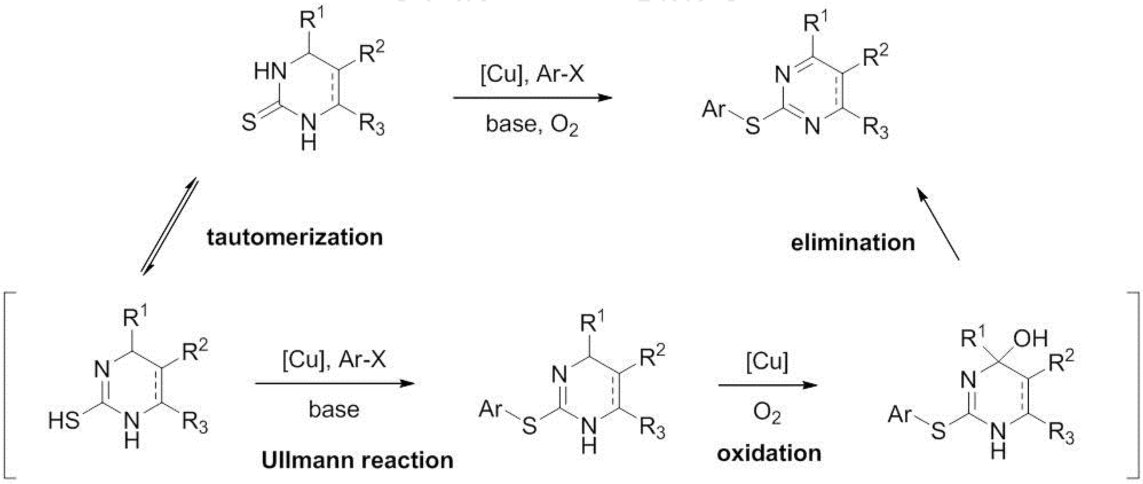
Copper-catalyzed aerobic oxidative C-S cross-coupling for conversion of cyclic thiourea to arylthiopyrimidines

이옥숙 손정훈*

충남대학교 화학과

For a facile accessibility and derivatization of novel pyrimidine compounds which are potentially valuable drug candidates, we devised Cu-catalyzed tandem reaction method for conversion of six-membered cyclic thioureas to arylthiopyrimidines via successive tautomerization, Ullmann reaction, oxidation and elimination. This reaction method was proved to be compatible with a wide range of 3,4-dihydropyrimidine-2(H)-thione core structures and aryl halides or biaryl iodonium salts as coupling partners.



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The novel conjugated alternating 2,2-bithiophene-3,3-dicarboximide containing polymers with different donor units: synthesis and photovoltaic application

백지연 서홍석[1,*]

부산대학교 자연과학대학/화학과 [1]부산대학교 화학과

The novel accepter unit, 4H-dithieno[3,2-c:2',3'-e]azepine-4,6(5H)-dione, was utilized and approved for the synthesis of the conjugated alternating polymers containing electron D-A pair for BHJ solar cells. The dithienoazepinedione, bithiophene imide (BTI) group, is an stylish electron deficient unit as it demonstrates strong electron-withdrawing disposition, and planar architecture. The polymer with benzodithiophene unit and linear dodecyl-BTI unit substituted with 2-octyldodecyl side chain was synthesized using Stille polymerization to produce P1. The novel polymer, P2, was synthesized by Suzuki polymerization of carbazole, thiophene and linear octyl-BTI unit to increase conjugation length. These polymers exhibited excellent good solubility and thermal stability. The spectra of P1 and P2 solid films show absorption bands with maximum peaks at P1:395, 538 P2:380, 491 nm and the absorption onsets by 652 and 634 nm, akin to band gaps of 1.90 eV, 1.96 eV, likewise. The best device with P1: PC71BM in ODCB with 2% DIO showed a VOC of 0.97 V, a JSC of 3.06 mA/cm2, and a FF of 0.49, which yielded PCE of 1.49%. and the P2:PC71PM (1:2) showed a VOC of 0.84 V, a JSC of 2.48 mA/cm2, and a FF of 0.36, which yielded PCE of 0.76%

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Photovoltaics Properties of BTI Based D-A Polymers for High Performance Polymer Solar cells

백지연 서홍석[1,*] 김주애[2]

부산대학교 자연과학대학/화학과 [1]부산대학교 화학과 [2]부산대학교 화학관 427호

Solution-processed bulk-heterojunction organic solar cells (BHJ OSCs) have substantially potential because of their high internal quantum efficiency and large-scale printing technique. The interest in solution-processable small molecular p-conjugated organic donors has been accelerating for BHJ photovoltaic applications in recent years, owing to the advantages of definite structure, facile purification, high purity and good photovoltaic performance reproduction. To develop innovative materials, novel computationally aided design strategy was made through the development of a new class of electron-transporting polymers by incorporating highly tailorable solubilizing groups into an electron-deficient core based upon the N-alkyl-2,2′-bithiophene-3,3′-dicarboximide unit (BTI). In comparison to other acceptor units, BTI units have the advantage of decreased steric encumberance achieved by placing the imide group at the center of BTI unit. The spectra of HS-5456 and HS-5467 solid films show absorption bands with maximum peaks at 368, 495 and 397, 517 nm corresponding to band gaps of 2.07 and 1.97 eV, respectively. The best device with HS-5456: PC71BM ratio of 1:3 showed a VOC of 0.91 V, a JSC of 3.93 mA/cm2, and a FF of 0.38, which yielded PCE of 1.36%. The highest PCE of HS-5457:PC71PM ratio of 1:4 showed solar cells reaches 1.08% with a VOC of 0.80 V, a JSC of 3.79 mA/cm2, and a FF of 0.36.

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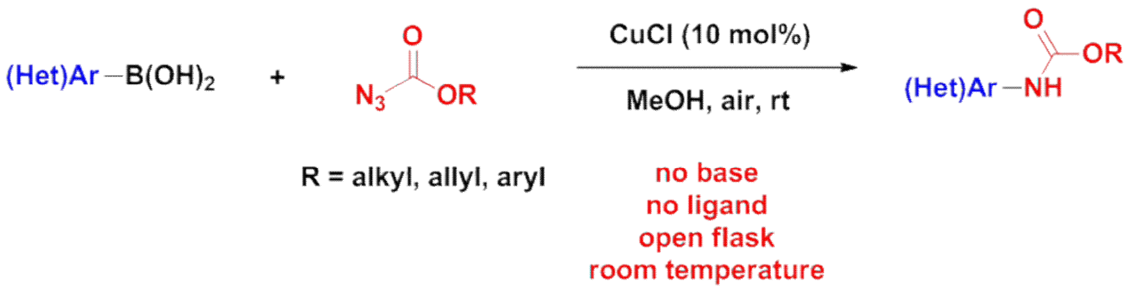
A New Approach to the Synthesis of N-Arylcarbamates

문수연 **KIMUBIN** 김원석*

이화여자대학교 화학 나노과학과

N-Arylcarbamate moiety is widely encountered in the structure of biologically active compounds. They are also valuable synthetic intermediates and are widely used for the synthesis of drug, urea derivatives and as protecting groups of amines in peptide synthesis. Even though these compounds are generally prepared from phosgene, phosgene derivatives or isocyanates in the presence of alcohols, these methods are not environmentally benign due to the use of toxic reagents and generation of by-products. Thus, various methods have been developed to synthesize N-arylcarbamates to avoid such drawbacks. Herein, we report a new approach to the synthesis of N-arylcarbamates employing boronic acids and azidoformate in an open flask at room temperature without any base, ligand, or additive. Various N-arylcarbamates were prepared with differing substitution and functional groups on both coupling partners to illustrate scope and tolerance of this mild and efficient methodology.



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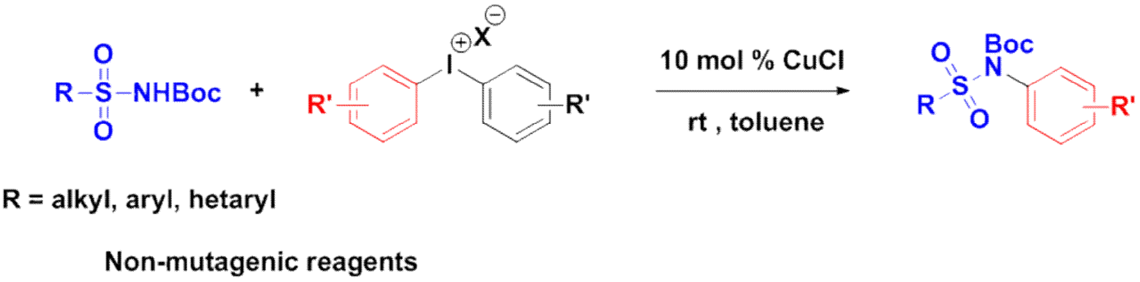
Studies on the Synthesis of N-Boc Arylsulfonamides Employing N-Boc Sulfonamide and Diaryliodonium Salt

고문지 최종희 김원석*

이화여자대학교 화학 나노과학과

N-Arylsulfonamides are a common moiety present in a large number of pharmaceutically interesting compounds. These arylsulfonamide derivatives have become popular in SAR studies in medicinal chemistry research since the early discovery of their anticancer, antibacterial, anticonvulsant and HIV protease inhibitory activities. Thus, various methods have been developed to synthesize N-arylsulfonamides. Herein, a mild and efficient method for the synthesis of N-Boc arylsulfonamide is demonstrated by using non-mutagenic N-Boc sulfonamide and diaryliodonium salt at room temperature. The reaction with N-Boc protected sulfonamides are shown to be cleaner and higher yielding than when using unprotected sulfonamides. In the presence of 10 mol% CuCl at room temperature, studies on the synthesis of N-Boc arylsulfonamides using various sulfonamides including alkyl, aryl and heteroaryl group and diaryliodonium salts are undergoing.



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Mild and efficient one-pot synthesis of phenylimidazo[1,2-a] pyridines

이슬기 박진균*

부산대학교 화학과

Imidazo[1,2-a] pyridines have been recognized as important building blocks for the biologically active compounds and N-heterocyclic carbene (NHC) precursors for transition metal catalysis. Therefore, there are many synthetic methods including palladium catalyzed coupling reactions and metal free condensations reaction. However, most of known methods require relatively long reaction time(overnight), high temperature(>60oC) and expensive starting materials. Our initial effort toward mild reaction condition found efficient one-pot metal free condensation of aminopyridines and aldehydes at room temperature within several hours.

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Small molecules consisting of phenanthrothiadiazole, benzimidazole and Benzodithiophene for bulk heterojunction solar cells

김주애 서홍석[1,*]

부산대학교 화학관 427호 [1]부산대학교 화학과

Recently, bithiophenes exposure a center aromatic ring was chosen as a model, since the planar benzodithiophene (BDT) unit has manufactured numerous high mobility semi-crystalline polymers, and the bordering thiophenes would lower steric hindrance and generate smaller dihedral angles with neighboring monomers. A new donor-acceptor small molecules incorporating benzodithiophene as the electron donating moiety have synthesized in organic solar cells with phenanthrothiadiazole(PT) as an electron accepting moiety. The DBDTPT and DBDTMBI, were synthesized by stille reaction and evaluated in OPVs. The optical band gaps of DBDTPT and DBDTMBI through the UV onset value of the λmax were 361 nm and 603 nm, respectively. The HOMO and LUMO levels of DBDTPT and DBDTMBI were exhibited at -5.46 and -3.65 eV and -5.85 and -3.84 eV, respectively. The small molecules have good thermal stability.

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The synthesis and characterization of various calix[4]pyrroles

김주연 이정태[1,*]

한림대학교 화학 [1]한림대학교 화학과

The human body is composed of more than 60 trillion cells and has a large number of anions. These anions have been recognized as essential elements to life. Because calix[4]pyrrole has widely been known as a receptor for these anions, intensive research has been conducted. In this study, the anion binding ability of various calix[4]pyrroles bearing different meso aryl groups has been compared using NMR titration. We studied the effect of a variation in the substituent of meso aryl on the bind strength using the Hammett equation.

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Synthesis and Characters of Copolymers Based on Dialkoxy-CF3 Substituted Benzimidazole for Organic solar cells

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부산대학교 화학관 427호 [1]부산대학교 화학과

Recently, conjugated polymers have been developed into useful materials for a variety of applications, including light-emitting diodes, organic solar cells and thin-film transistors (TFTs). Inserting fluorine atoms on acceptor units can improve the key factors of PCE including open-circuit voltage (VOC), short-circuit current density (JSC), and fill factor (FF). There are for a new processable, high-molecular-weight, highly conjugated benzimidazole derivatives, HS-5481, HS-5482, HS-5484 and HS-5485. In this article, we report the characterization of the newly synthesized polymer HS-5481, HS-5482, HS-5484 and HS-5485 that were synthesized by the palladium-catalyzed Stille and Suzuki polymerization. The UV-vis absorption of HS-5481 and HS-5482 exhibited maximum peak at 365 and 727 nm, 410 and 727 nm in the film state. HS-5484 and HS-5485 exhibited maximum peak at 440 and 679, 397 and 611 nm in the film state. The absorption onset wavelength of HS-5481, HS-5482, HS-5484 and HS-5485 were observed for 809, 828, 843 and 732 nm in solution, which corresponds to optical band gaps of 1.51, 1.48, 1.47 and 1.69 eV. The electrochemical band gaps, calculated from CV data, are about 1.68~1.98 eV, a bit more higher the electrochemical bandgaps estimated from the onset wavelengths of the absorption spectra, respectively. The device founded on the polymers HS-5481, HS-5482 showed VOC of 0.41 , 0.69 V, JSC of 0.54, 2.62 mA/cm2, and FF of 0.36, 0.4 giving a PCE of 0.08%, 0.72%.

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발표종류: 포스터, 발표일시: 수 16:00~19:00

Conjugated polymers consisting of pyrrolo[3,2-b]pyrrole (i-DPP) as donor materials for organic solar cell

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부산대학교 화학관 427호 [1]부산대학교 화학과

Among the D-A conjugated polymer's acceptor units, pyrrolo[3,2-b]pyrrole-2,5-dione derivatives have been the most extensively used due to strong the electron withdrawing properties. Pyrrolo[3,2-b]pyrrole-2,5-dione element, structural isomer of the branded pyrrolo[3,4-c]pyrrole-1,4-dione (i-DPP), is maked commencing the structure of firm synthetic pigment. The novel low-band gap conjugated polymer with pyrrolo[3,2-b]pyrrole-2,5-dione, carbazole and thiophene was synthesized by Suzuki polymerization to produce P1. The solid film of P1 shows absorption band through maximum peaks at 374 and 548 nm, and the absorption onset at 679 nm, matching to band gap of 1.83 eV. The hole mobility of P1 is 2.2×10-5 cm2/Vs. The device founded on the polymer:PCBM (1:2) blend without thermal behavior showed VOC of 0.82 V, JSC of 6.28 mA/cm2, and FF of 0.39, giving a PCE of 2.00%.

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발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis and characterization is based on pyrrolo[3,4-c]pyrrole-1,4-dione for organic solar cells

김주애 서홍석[1,*]

부산대학교 화학관 427호 [1]부산대학교 화학과

Organic solar cells have development of new materials is compulsory to enhance the report of the solar spectrum and the absorption coefficients, which can improve the lower power conversion efficiency and lower photo current as compared to the cases of inorganic solar cells. The polymer of pyrrolo[3,2-b]pyrrole-2,5-dione, exhibits much attention as the electron poor unit for the production of electron-donor material for organic solar cells. Pyrrolo-[3,2-b]pyrrole-2,5-dione unit, region isomer of the known pyrrolo[3,4-c]pyrrole-1,4-dione, is originated from the structure of stable synthetic pigment. The organic low band gap molecules with pyrrolo-[3,2-b]pyrrole-2,5-dione, thiophene and triphenyl amine units were synthesized using Suzuki reaction to generate SM-B, SM-M and SM-H. The spectrum of SM-B confirms absorption band with maxima of 356 and 517 nm, and the onset peak at 667 nm, matching to band gap of 1.86 eV, respectively. The device blending SM-B and PC71BM (1:4) explained a VOC of 0.79 V, JSC of 6.04 mA/cm2, and a FF of 0.33, exhibits power conversion efficiency of 1.56%.

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Efficient deep-blue OLEDs using nondoped system with imidazole-triphenylamine derivatives

정성진 홍종인*

서울대학교 화학부

Deep-blue fluorescent organic light-emitting diodes (FLOLEDs) possessing high efficiency and pure Commission Internationale de l’Eclairage (CIE) chromaticity coordinates are a prerequisite for full-color displays and lighting devices. Nonetheless, because of the wide bandgap of blue emitters, only a few examples of high-performance blue FLOLEDs have been reported, in contrast to red and green FLOLEDs. A nondoped system has an advantage in that it has a simple device structure that employs only a single emitting material without using a complicated host?dopant codeposition process. Two triphenylamine-substituted benzimidazole derivatives were designed and synthesized for use as efficient deep-blue emitters in nondoped FLOLEDs. Nondoped FLOLED devices fabricated using 4′,4″-(1H-benzo[d]imidazole-1,2-diyl)bis(N,N-diphenylbiphenyl-4-amine) (T2B) as a blue emitter exhibited an external quantum efficiency of 4.67% with CIE coordinates of (0.15, 0.08).

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

A Synthetic Carrier Capable of Selectively Transporting Potassium Chloride across a POPC Membrane

이지현 정규성*

연세대학교 화학과

We have designed and prepared an ion-pair receptor that contains two heterotopic binding sites, an 18-azacrown-6 for potassium and a urea with a hydroxyl arm for chloride. As anticipated, this molecule strongly binds potassium chloride and selectively transports the salt by a symport mechanism across a POPC membrane. Binding properties are investigated in 1H NMR spectroscopy, showing strong cooperative binding as a contact ion-pair between the bound potassium ion and chloride ion, which results in large enhancement of the binding affinity of the salt relative to the individual binding of each ion, potassium or chloride. Details will be described in the presentation.

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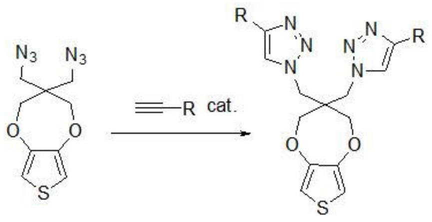
발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis and characterization of 3,4-propylenedioxythiophene (ProDOT) derivatives via click chemistry

정규관* 박여정[1]

전북대학교 과학교육학부 [1]전북대학교 화학교육과

3,4-Propylenedioxythiophene (ProDOT) and its derivatives are widely used monomers for electrically conducting polymers. Azide-functionalized ProDOT derivatives were synthesized and 1,3-dipolar cycloaddition upon it gave a variety of ProDOT derivatives as useful monomers for conducting polymers.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Fluorescence Chemosensor for Fluoride Anion with Coumarine Bypiridine Derivative

이환석 윤희상 남계춘*

전남대학교 화학과

The studies of chemosensors toward F^- anion are quite intriguing because of its beneficial effects in human physiology. Also, fluoride is interest due to its established role in dental care and osteoporosis. However, an excess of fluoride ion can lead to fluorosis. Therefore, developments of reliable sensors for fluoride ion are needed for environment and human health care. Among anion receptors, colorimetric and fluorescent chemosensors are important because they provide high sensitivity and convenience for monitoring the anion recognition.[1] Especially, coumarine are a particularly elegant basis for ratiometric based optical sensors. Here, we report a novel coumarine bipyridine chemosensor 1 with a specific optical response to fluoride ion. In pursuit of a selective fluoride chemosensor, a coumarine bipyridine derivative 1 was synthesized, and its anion binding properties were investigated by ^{1}H NMR, UV-vis spectroscopy, color changes, and fluorescence titration analysis.

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Calix[4]pyrrole carrying crown ether moiety at meso-positions as novel heteroditopic ion-pair receptor model

이창희* 하민지

강원대학교 화학과

Calix[4]pyrroles possessing benzocrown moiety at diametrical meso-positions in cis-conformation have been synthesized and characterized. The ion pair binding study of the synthesized hosts displayed interesting recognition properties as well as selectivity. The deep binding pocket strongly interacts with anion through hydrogen bonding and anion-pi interaction, while the adjacent crown ether moiety interact with counter cation in cooperative way. The receptor displayed different selectivity depending on the nature of applied ion-pairs. The extensive ion binding studies confirmed that the synthesized receptors form stable complexes with various metal salts including amino acids in polar organic media. The detailed binding studies and spectroscopic changes associated with ion binding will be presented.

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Unusual Trimerization of Aldehydes via Metal-Free Aerobic Oxidative Esterification of Aldehydes with Benzoin Products in the Presence of Cyanide in DMSO

김유진 천철홍*

고려대학교 화학과

A new, efficient, and mild protocol for the synthesis of trimers from aldehydes has been developed under ambient conditions in presence of sodium cyanide. The efficiency of this transformation showed strong dependence on the choice of solvent and the amount of cyanide. Under the optimized conditions, various aromatic aldehydes afforded the desired trimeric compounds in moderate to high yield depending on the nature of aldehydes. Furthermore, Although the benzoin products was not directly converted into other useful products, the resulting trimers could be easily converted into other useful products, such as oxazole and benzofuran products, which demonstrated the usefulness of this transformation. Mechanistic studies revealed that this reaction proceeds via benzoin condensation, followed by aerobic oxidative esterification of aldehydes with the resulting benzoin product.

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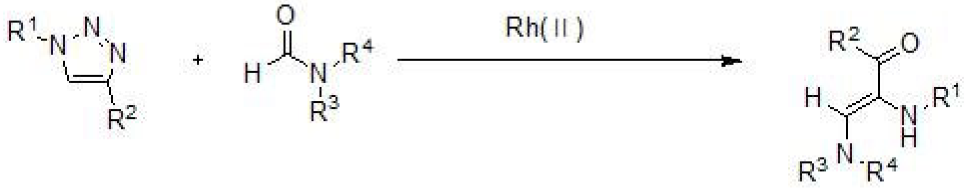
발표종류: 포스터, 발표일시: 수 16:00~19:00

Rhodium catalyzed Denitrogenative Coupling reaction of Triazoles with DMF

정다정 전현지 이상기[1,*]

이화여자대학교 화학나노과학과 [1]이화여자대학교 화학/나노과학과

Rhodium(Ⅱ) azavinyl carbenes, generated from triazoles, involve critical potential to undergo various chemistry with characteristic reactivity. Herein, we present an unprecedented rhodium-catalyzed denitrogenative coupling of N-sulfonylated triazoles, which can readily prepared by copper-catalyzed click coupling of azides and 1-alkynes, with DMF, which in turn to be a highly efficient novel method for stereoselective synthesis of cis-diamino substituted conjugated carbonyl compounds.



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The role of the water in synthesis of benzimidazoles via metal-free aerobic oxidation

이예솔 천철홍*

고려대학교 화학과

Benzimidazoles are common building blocks found in biologically and therapeutically active compounds, natural products and material science. Thus, the development of efficient synthetic methods to access these important compounds has been extensively investigated. One of the conventional methods for the synthesis benzimidazoles is oxidative cyclization which is starting from o-phenylenediamine and aldehyde through imine intermediates in presence of strong oxidants. Recently we have developed the novel one-pot protocol via metal-free aerobic oxidation. During this investigation, we found that water is the key factor of oxidative cyclization. Based on this finding, we have developed highly environmental benign protocol for the synthesis of benzimidazoles in either wet organic solvents or protic solvents. In addition, this protocol can be extended to the synthesis of benzimidazoles bearing oxidation-labile functional group such as boronic acid.

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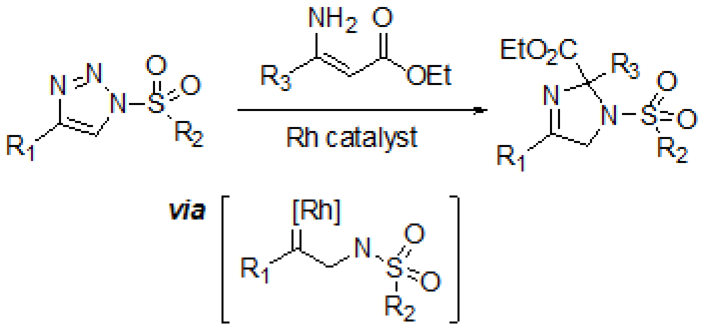
A New Approach for the Synthesis of Imidazole Derivatives from N-Sulfonylated Triazoles via Rhodium(Ⅱ) Azavinyl Carbene

전현지 정다정 이상기[1,*]

이화여자대학교 화학나노과학과 [1]이화여자대학교 화학/나노과학과

Nitrogen-containing heterocycles, especially imidazoles are ubiquitous in both natural products and pharmaceuticals. , Accordingly the development of new synthetic method for this class of heterocyclic compounds is highly important. Herein, we present a new strategy for the synthesis of imidazole derivatives by reaction of the rhodium(Ⅱ) azavinyl carbene, generated in situ from N-sulfonyl-1,2,3-triazole, with enaminoesters



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발표종류: 포스터, 발표일시: 수 16:00~19:00

Fluorescent Off-On Chemosensor for Fluoride Ion with Pyrene Based on Triphenylphosphine

윤희상 이환석 남계춘*

전남대학교 화학과

The supramolecular chemistry of anions provides a means to sense and manipulate anions in their many chemical and biological roles. Anions are ubiquitous and they have major roles in the natural world. In particular, the studies of F^- anion are quite intriguing because of its beneficial effects in human physiology. Also, fluoride is interest due to its established role in dental care and osteoporosis. However, an excess of fluoride ion can lead to fluorosis. Therefore, the development of reliable sensors for F^- is needed for environment and human health care. Fluorescent chemosensors can be effectively used as a tool to analyze and classify such roles of charged chemical species in living system as well as to measure the amount of ions from the sources contaminated with them. Among anion receptors, colorimetric and fluorescent chemosensors are important because they provide high sensitivity and convenience for monitoring the anion recognition. The salt type derivative was obtained successfully by the reaction of triphenylphosphine with pyrene derivative. The binding properties of triphenylphosphine derivative investigated with ^{1}H-NMR and fluorescence titration methods with various anions.

일시: 2014년 4월 16~18일(수~금) 3일간
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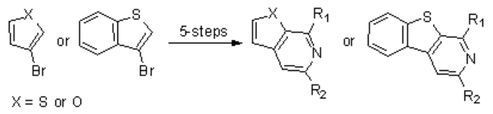
발표분야: 유기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

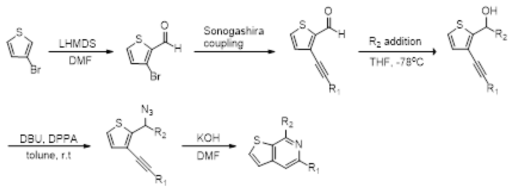
Synthesis of Variously Disubstituted Pyridine-fused Ring Compounds via Intramolecular Cyclization without Metal Catalyst

이재탁 이원구* 이호규 이준호 하현준[1],*

서강대학교 화학과 [1]한국외국어대학교 화학과

Many substituted pyridines and pyridine-fused compounds show biologically activities. Therefore, there has been much efforts for the syntheses of those heterocycles using efficient and also environmentally benign process. In our previous work, we successfully synthesized substituted azaindoles by intramolecular cyclization reaction of azide and acetylene substituted pyrrole without any catalyst. We found that disubstituted thienopyridine, benzothienopyridine and furopyridine could be efficiently synthesized from thiophene, benzothiophene and furan without catalyst by same method.





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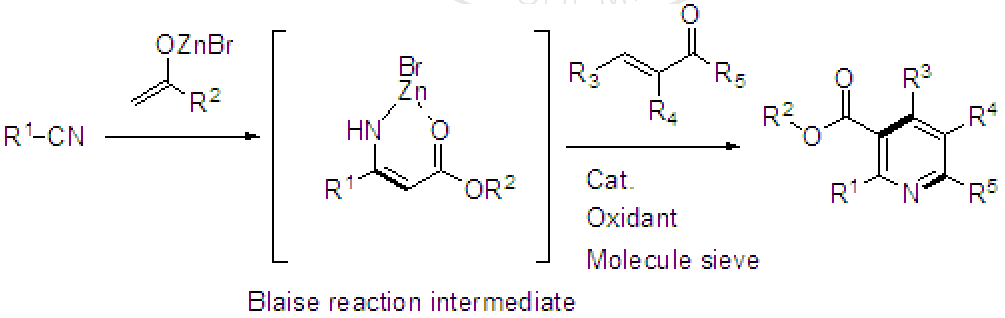
발표코드: **ORGN.P-800**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Tandem One-Pot Synthesis of Highly Substituted Pyridines using the Blaise Reaction Intermediate

XUAN ZI 이상기[1,*]

이화여자대학교 화학.나노학과 [1]이화여자대학교 화학/나노과학과

The pyridine moieties are found in many biologically relevant compounds, which have various activities such as anitiviral(HIV), anitimicrobial, anticancer, and protein kinase inhibition activity. The synthetic methodologies of this heterocycle mainly rely on condensation of amines and carbonyl compounds or cycloaddition reactions. In the course of our ongoing study on tandem use of the Blaise reaction,we found an operationally simple, scalable, and flexible procedure for constructing pyridine rings with controllable substitution patterns around the pyridine core through a tandem reaction of Blaise reaction intermediate with α,β-unsaturated carbonyl compounds.



일시: 2014년 4월 16~18일(수~금) 3일간
장소: 일산KINTEX
발표코드: **ORGN.P-801**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Asymmetric synthesis of Biologically Active Pyrrolidine Alkaloids from Chiral Aziridine-2-carboxylate

이재덕 양지은* 하현준* 이원구[1,*]

한국외국어대학교 화학과 [1]서강대학교 화학과

Pyrrolidine alkaloids were natural products which exhibit a wide range of potent biological and pharmacological activities. Methyl-(2*S*)-acetyl methyl pyrrolidin-5-one as key intermediate was prepared from chiral aziridin-2-carboxylate through methylative aziridine ring opening reaction with cyanide nucleophile followed by reductive cyclization. Methylation and the subsequent selective reductions afforded the asymmetric synthesis of (-)-hygroline and (-)-pseudohygroline, alkylation and lactam activation afforded the asymmetric synthesis of (-)-ferruginine and methylecgonidine.

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발표코드: **ORGN.P-802**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Unprecedented C2-Olefination of *N*-Substituted Indole and Pyrroles via Rh-catalyzed oxidative C-C bond formation and C-N bond cleavage

신영미* 박지혜 한상일

성균관대학교 약학과

The indole nucleus is a ubiquitous structural motif found in bioactive natural products, pharmaceuticals, functional materials, and agrochemicals. Thus the efficient synthesis and functionalization of indoles have been of considerable interest in organic and medicinal chemistry. In particular, transition-metal-catalyzed cross-coupling of indoles and aryl halides is one of the most sustainable protocols for the functionalization of indoles. Since the pioneering efforts of Fujiwara and Moritani, remarkable progress has been made on the oxidative Heck coupling between indoles and olefins under palladium catalysis via a twofold C-H bond cleavage. Due to the electrophilic nature of the organometallic species involved in the coupling reaction, the reaction occurs preferentially at the more electron-rich C3 position of the indole ring. Therefore, the highly selective C2-olefination of 2,3-unsubstituted indoles has been an intensive research area to override the inherent selectivity of indoles. For instance, Gaunt described the regioselective Pd-catalyzed intermolecular C2- or C3-alkenylation of free (NH)-indoles by employing different solvents and additives. Satoh and Miura disclosed the Pd(II)- catalyzed C-H alkenylation and subsequent decarboxylation protocol of indole-3-carboxylic acids to afford exclusively C2-alkenylated indoles, where the carboxyl group blocks the C3-position and acts as a removable directing group. Recently, Carretero reported the highly efficient Pd-catalyzed C2-selective olefinations of indoles and pyrroles assisted by a removable *N*-(2-pyridyl)sulfonyl group. In contrast to the vast majority of documents on the palladium-catalyzed olefinations, the indolic C-H olefinations using rhodium or ruthenium catalysts, which often allow higher selectivities and broad substrate scope, have been much less explored. For example, Glorius first reported a single example of Rh-catalyzed C2-olefination of *N*-acetyl indoles. Prabhu demonstrated Ru-catalyzed oxidative C2-alkenylation of indoles using the *N*-

benzoyl directing group. Recently, Li and Wang and Song, respectively, reported Rh(III)- and Ru(II)-catalyzed oxidative couplings between indoles containing a *N*,*N*-dimethylcarbamoyl group and olefins to afford C2-alkenylated indoles In conclusion, we developed a novel strategy for the formation of C2-functionalized free (NH)-indoles and free (NH)-pyrroles via the rhodium(III)-catalyzed oxidative alkenylation of *N*-arylcarbamoyl indoles and pyrroles with olefins and subsequent cleavage of a protection group. Further applications to the synthesis of biologically active compounds and a more detailed mechanistic investigation are in progress.

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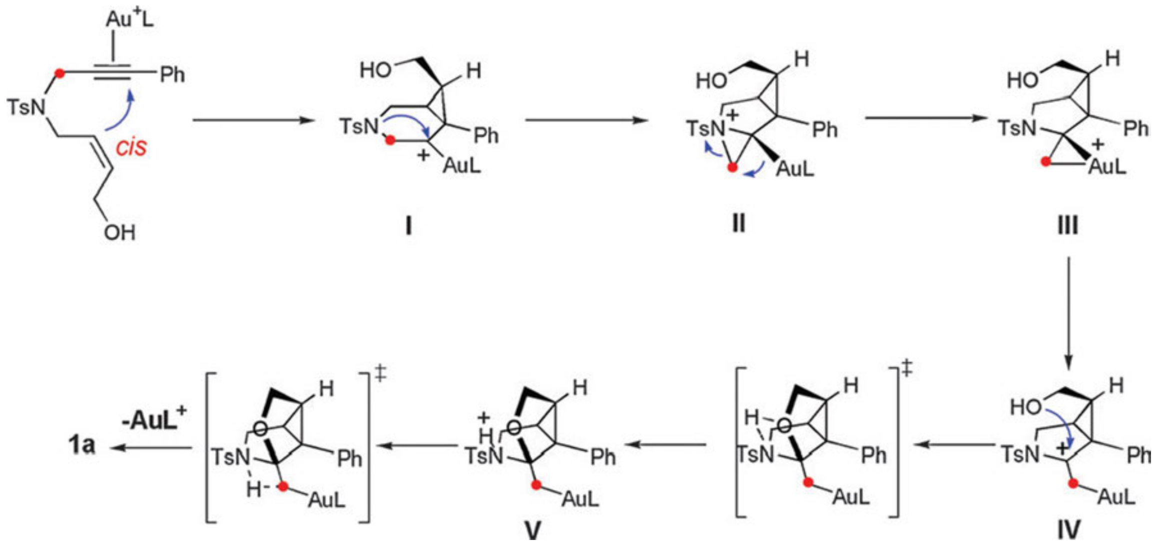
발표분야: 유기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Theoretical Investigation on the Reaction Mechanism of Gold(I)-Catalyzed Cyclosiomerization of Alkynyl Hydroxyallyl Tosylamides to 4-oxa-6-azatricyclo[3.3.0.0^{2,8}]octanes

정대로 강윤경*

상명대학교 화학과

Developing a new synthetic method via transition metal-catalyzed reaction is one of the major research areas in organometallic chemistry. Cycloisomerization reactions of N-tethered enyne have been of great interest due to their wide applicability toward the synthesis of variety of cyclized compounds. Recently, Chung and coworkers have reported Au(I)-catalyzed cycloisomerizations of alkynyl hydroxyallyl tosylamides, which gave a totally new 4-oxa-6-azatricyclo[3.3.0.0^{2,8}] compound. Other metal catalysts that include Rh, Ir, Pd, and even Au metals have only given Alder-ene type products. Here we investigated the reaction mechanism that rationalizes the production of unprecedented 4-oxa-6-azatricyclo[3.3.0.0^{2,8}] compound by using a density functional theory (DFT) calculation. The reaction starts from the 6-*endo-dig* cyclization (I), followed by a transannulation between the nitrogen atom and the carbon atom attached to the gold cation (II). Shift of the catalyst moiety leads to a formation of III which may equilibrate with IV. Because of the significant carbocationic character at the alkynyl carbon adjacent to the N-Ts group in IV, a nucleophilic addition of the hydroxyl oxygen occurs to give V. Proton transfer followed by protodemetalation in V affords the product and regenerates the gold(I) catalyst in the catalytic cycle.


Au+L
TsN
Ph
cis
OH
HO
H
TsN
Ph
+
AuL
I
II
III
IV
V
‡
-AuL+
1a
H
O

일시: 2014년 4월 16~18일(수~금) 3일간
장소: 일산KINTEX
발표코드: **ORGN.P-804**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Highly Stable, Water-dispersible Metal Nanoparticle-decorated Polymer Nanocapsules and Their Catalytic Applications

HASSANZAHID 윤경원[1] 김기문[1,*]

기초과학연구원 복잡계 자기조립 연구단 [1]포항공과대학교 화학과

A facile synthesis of highly stable, water-dispersible metal nanoparticle-decorated polymer nanocapsules (M@CB-PNs: M = Pd, Au, and Pt) was achieved in a simple two-step process employing a polymer nanocapsule (CB-PN) made of cucurbit[6]uril (CB[6]) and metal salts. The CB-PN serves as a versatile platform where various metal nanoparticles (NPs) with a controlled size can be introduced on the surface and stabilized to prepare new water-dispersible nanostructures useful for many applications. The Pd nanoparticles on CB-PN exhibit high stability and dispersibility in water, as well as excellent catalytic activity and recyclability in carbon-carbon and carbon-nitrogen bond formation reactions in aqueous media suggesting potential applications as a green catalyst. Details of this work will be presented.

Highly Stable, Water-dispersible Metal Nanoparticle-decorated Polymer Nanocapsules and Their Catalytic Applications

Zahid Hassan[1], Gyeongwon Yun[1,2], and Kimoon Kim[1,2]*
[1]Center for Self-assembly and Complexity, Institute for Basic Science (IBS), Pohang, Republic of Korea
[2]Department of Chemistry, Pohang University of Science and Technology (POSTECH), Pohang, Republic of Korea

Abstract: A facile synthesis of highly stable, water-dispersible metal nanoparticle-decorated polymer nanocapsules (M@CB-PNs: M = Pd, Au, and Pt) was achieved in a simple two-step process employing a polymer nanocapsule (CB-PN) made of cucurbit[6]uril (CB[6]) and metal salts. The CB-PN serves as a versatile platform where various metal nanoparticles (NPs) with a controlled size can be introduced on the surface and stabilized to prepare new water-dispersible nanostructures useful for many applications. The Pd nanoparticles on CB-PN exhibit high stability and dispersibility in water, as well as excellent catalytic activity and recyclability in carbon-carbon and carbon-nitrogen bond formation reactions in aqueous media suggesting potential applications as a green catalyst. Details of this work will be presented.

일시: 2014년 4월 16~18일(수~금) 3일간
장소: 일산KINTEX
발표코드: **ORGN.P-805**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Heavy Atom-bearing Tripod Amphiphiles for Membrane Protein Solubilization and Stabilization

배형은 채필석[*]

한양대학교 생명나노공학과

Integral membrane proteins are extremely stable in their native membranes, but tend to aggregate and denature when solubilized with detergent molecules for their structural and functional study and necessitating the addition of detergent molecules to separate the hydrophobic portion of membrane proteins from an aqueous medium. Here, we introduced a new TPA with a heavy atom, iodine. We enhance the hydrophobic part , strong x-ray scattering positon, and found that it is superior DDM, the most succeessful conventional detergent, and TPA-2, a previous described TPA with branch diglucoside, in therms of membrane protein solubilization and stabilization efficacy.

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

A Novel Class of Amphiphiles Bearing Adamantane Groups for Solubilization and Stabilization of Membrane Proteins

DASMANABENDRA 채필석[1,*]

한양대학교 bionano engineering [1]한양대학교 생명나노공학과

Integral membrane proteins play important roles in controlling the flow of molecules and information across membranes. Conventional detergents, used to resolve the incompatibility between the large hydrophobic surfaces on membrane proteins in their native forms and polar solvent molecules, often causes protein aggregation and denaturation. Therefore, for advancement of membrane protein research, development of novel detergents is necessary. Here, we introduce several adamantane-containing amphiphiles and evaluated for their capability of protein solubilization and stabilization. Our study reveals the superiority of some of these agents toward protein solubilization efficiency relative to the conventional detergents.

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

Hydrophobic Variants of Glucose-neopentyl Glycol (GNG) Amphiphiles for Membrane Protein Study

조경호 채필석*

한양대학교 생명나노공학과

Our understanding of membrane protein structures and their functions is hampered by the difficulties associated with handling these bio-macromolecules. Amphipathic agents, called detergents, are widely used for the determinations of membrane protein structures. Here, we present several hydrophobic variants of GNG amphiphiles evaluated for a large, multi-subunit membrane protein assembly. These variants displayed enhanced behaviors in terms of membrane protein solubilization and/or stabilization efficacy relative to previously-reported GNG agents and conventional detergents. Importantly, the present study enabled us to propose an important detergent structure-property relationship which provides a useful guideline for new detergent design.

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

Highly Enantioselective Extraction of Underivatized Amino Acids by the Uryl-Pendant Hydroxyphenyl-Binol Ketone

ChenQian 김관묵[1,*]

이화여자대학교 화학나노과학과 [1]이화여자대학교 화학과

Pure enantiomeric amino acids attracted significant interests because they are widely used in basic peptide and pharmaceutical industries. Enantioselective liquid-liquid extraction (ELLE) is one of promising extraction processes applied in the chiral resolution of amino acids. This method has great advantages in industrial application due to low energy consumption, continuous recycling and easy scaling up. Here our group successfully synthesized the hydroxyphenyl chiral ketone, which shows high selectivities as a chiral extractant in the ELLE for general underivatized amino acids. The multiple hydrogen bonds formed in the imine of the ketone with an amino acid reinforce the rigidity, and result in the different stability between the imine diastereomers. The amino acids obtained after the hydrolysis of the imine in methanol have enantiomeric excess (ee) values of over 97%. The ketone could have been perfectly recycled and entered into a new extraction cycle.

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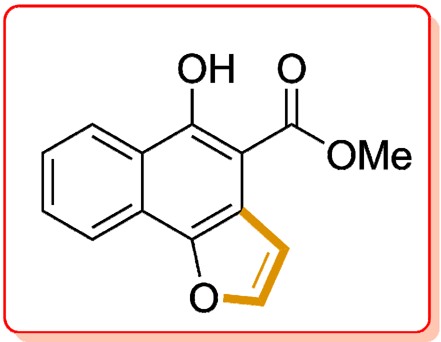
장소: 일산KINTEX
발표코드: **ORGN.P-809**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis and Biological Evaluation of Furomollugin and Its Analogues

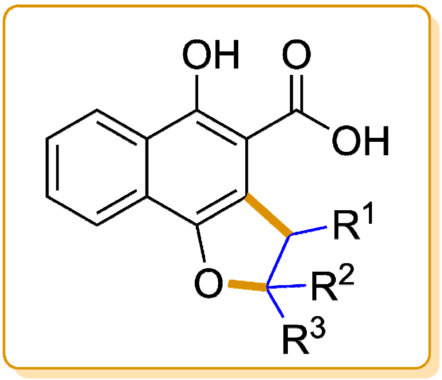
CAIHONGYUN 하립개 이용록*

영남대학교 화학공학부

Diverse furomollugin (3) and its analogues (11 - 22) were synthesized in high yields via CAN-catalyzed formal [3+2] cycloaddition as a key step. The in vitro antioxidant activities of synthesized compounds were determined by analyzing radical scavenging activities for 1,1-diphenyl-2-picrylhydrazyl (DPPH), nitric oxide (NO), and hydrogen peroxide (H_2O_2) assays. The results showed that the synthesized furomollugin analogues had effective antioxidant power. Dihydronaphthofurans with 2-alkyoxy or 2-aryl group were the most potent radical scavengers in DPPH assay. Moreover, the antibacterial activities of those compounds were also evaluated and the highly active compounds were selected for further determination of minimal inhibitory concentrations (MICs). Compound 19 (MIC = 2 μg/mL) was found to be highly active against the gram-negative bacteria *E. coli* (KCTC-1924) than the Ampicillin standard (MIC = 4 μg/mL). Compound 22 (MIC = 0.5 μg/mL) inhibited gram-positive bacteria *S. aureus* (KCTC-1916) growth as effectively as Ampicillin (MIC = 0.5 μg/mL).



Furomollugin (**3**)



Furomollugin analogues (**11-22**)

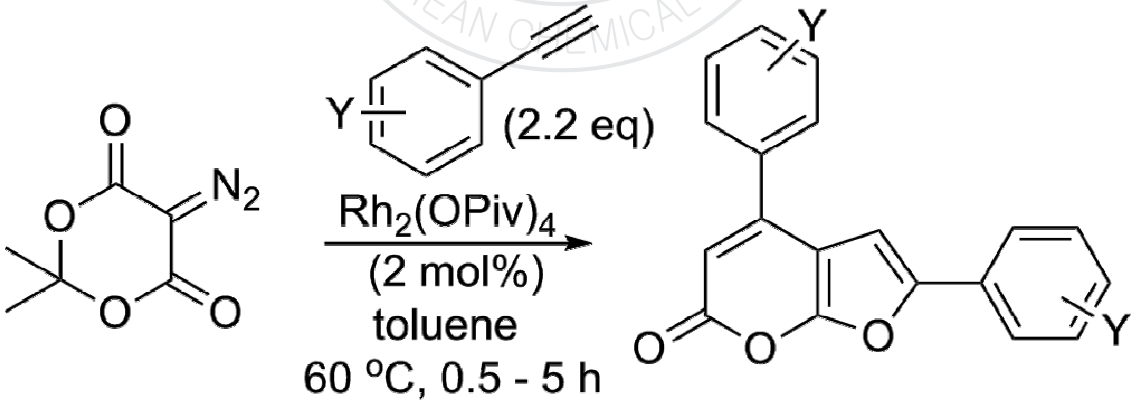
일시: 2014년 4월 16~18일(수~금) 3일간
장소: 일산KINTEX
발표코드: **ORGN.P-810**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Rhodium (II)-Catalyzed Cascade Reactions of Diazo Compound for the Synthesis of Biologically Interesting Furo[2,3-b]pyran-6-ones

KHANALHARIDATTA 소마이마가크리쉬나 이용록*

영남대학교 화학공학부

We present herein an efficient synthesis of biologically interesting furo[2,3-b]pyran-6-ones by rhodium(II)-catalyzed reactions of diazo compound and a variety of ethynyl compounds. These reactions provide a rapid approach for synthesizing a variety of furo[2,3-b]pyran-6-one derivatives in one-pot cascade reactions of metal carbenoid reaction/ ketene formation /[2+2]cycloaddition /subsequent ring expansion. This methodology has the advantages of mild reaction conditions, efficient catalytic ability, and simple experimentation requirements.



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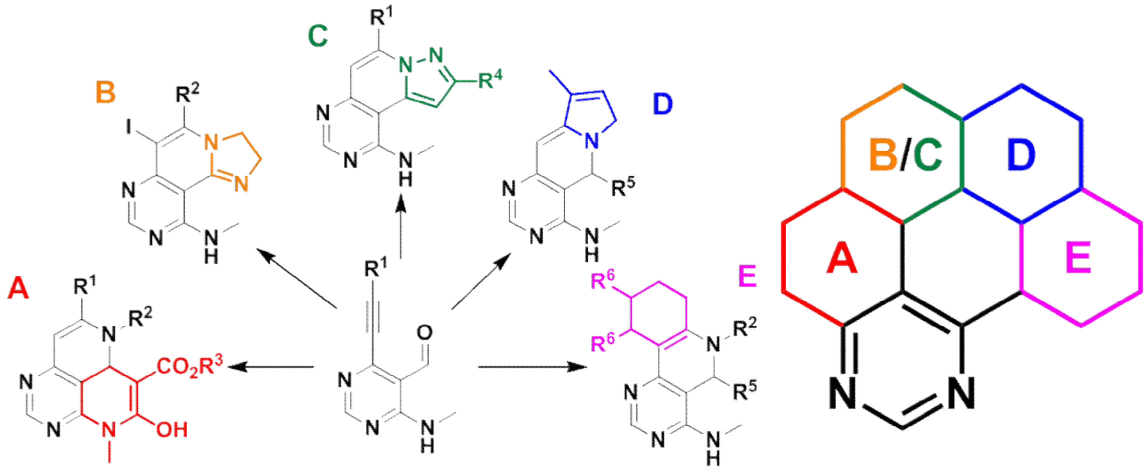
발표분야: 유기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Privileged Substructure-Based Diversity-Oriented Synthesis Pathway for Diverse Pyrimidine-Embedded Polyheterocycles

김희준 박승범*

서울대학교 화학부

Facile fabrication of a structurally diverse small-molecule library plays a crucial role in drug discovery and chemical biology. In particular, the unbiased collection of small molecules has become an inevitable resource because it can provide a unique opportunity for the identification of novel chemical entities from phenotype-based screening, which is the leading approach for the development of first-in-class drugs. Diversity-oriented synthesis (DOS) plays an indispensable role to access the unexplored molecular frameworks with maximum structural and stereo-chemical diversity. Along with this endeavor, we proposed a privileged substructure-based DOS (pDOS) for the efficient generation of distinct polyheterocyclic core skeletons embedded with privileged substructures. Pyrimidine has been extensively explored in synthetic and medicinal chemistry owing to its unique mimicking of nucleosides and hydrogen bonding ability with nucleic acids in biological systems. We have developed a new pDOS strategy with pyrimidine as the privileged substructure. Five core skeletons were synthesized by silver- or iodine-mediated cascade cyclization with various amines under different reaction conditions. The resulting discrete scaffolds consist of unique pyrimidine-embedded polyheterocycles fused with different ring sizes and orientation. The molecular diversity of each scaffold was successfully confirmed by a structural alignment of energy-minimized 3D conformers, shape diversity studies using PMI analysis, and PCA analysis. This pDOS strategy allows the fabrication of unique polyheterocycles along with a wide spatial coverage around pyrimidine as the privileged substructure that ensures high potential for molecular interactions with biopolymers in a selective and specific manner.


C
R1
N
N
R4
B
R2
I
D
N
N
N
N
N
H
A
R1
R2
CO2R3
OH
E
R6
R6
R5
O
B/C
D
A
E
N
N

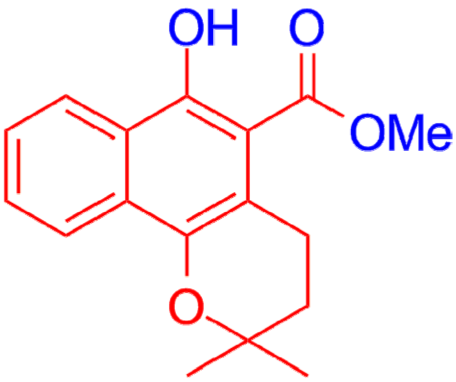
일시: 2014년 4월 16~18일(수~금) 3일간
장소: 일산KINTEX
발표코드: **ORGN.P-812**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis of Novel Mollugin Derivatives and Their Evaluation ofBiological Activities

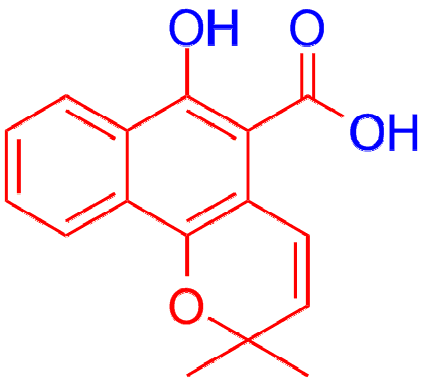
BARALEKRAJ AKBERALIIDHAYADHULLA 이용록*

영남대학교 화학공학부

Novel and diverse mollugin analogues were synthesized and screened for their in vitro antioxidant activities, using a 2,2-diphenyl-1-picrylhydrazyl (DPPH) assay method, and for their in vitro antibacterial activities against Escherichia coli (KCTC-1924) and Staphylococcus aureus (KCTC-1916) bacterial strains. The antioxidant activities of synthesized mollugin (1), 3,4-dihydromollugin(2) and their analogues 3-12 were compared with butylated hydroxytoulene (BHT), and the antibacterial activities of the synthesized compounds 2 were compared with ciprofloxacin. The synthesized compound exhibited potent inhibitory (95.62% at 100 ?g/mL; IC50 value of 0.15 ?g/mL) versus the BHT standard (74.80% at 100 ?g/mL; IC50 value of 2.13 ?g/mL) in the DPPH assay and compound 3 showed better bacterial growth inhibition against Staphylococcus aureus than the ciprofloxacin standard.



Compound **2**



Compound **3**

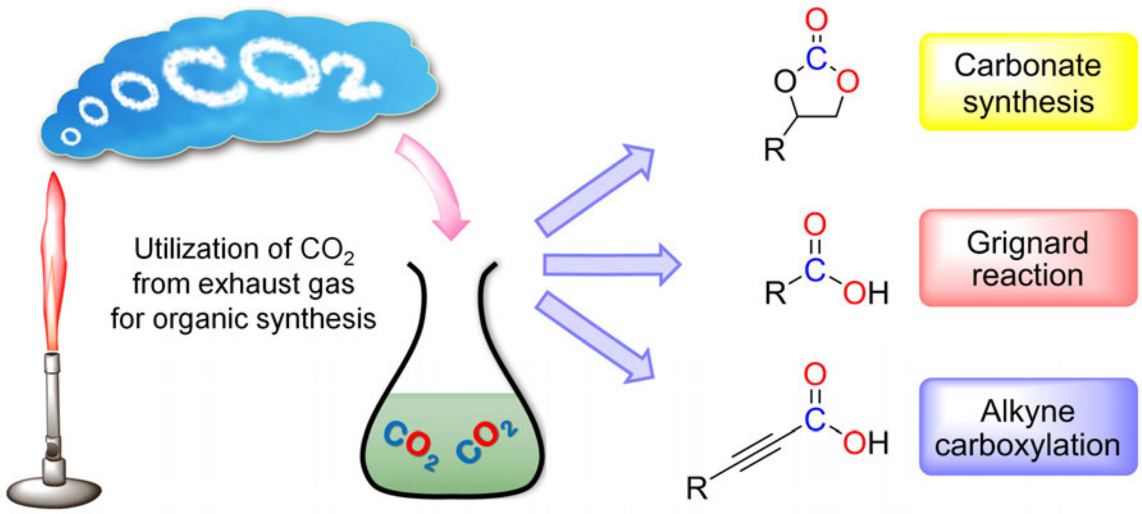
일시: 2014년 4월 16~18일(수~금) 3일간
장소: 일산KINTEX
발표코드: **ORGN.P-813**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Carbon Dioxide Capture and Use: Organic Synthesis Using Carbon Dioxide from Exhaust Gas

김승효 홍순혁[1,*]

서울대학교 화학부 [1]서울대학교 화학과

A carbon capture and use (CCU) strategy was applied to organic synthesis. Carbon dioxide (CO2) captured directly from exhaust gas was used for organic transformations as efficiently as hyper-pure CO2 gas from a commercial source, even for highly air- and moisture-sensitive reactions. The CO2 capturing aqueous ethanolamine solution could be recycled continuously without any diminished reaction efficiency.



일시: 2014년 4월 16~18일(수~금) 3일간

장소: 일산KINTEX

발표코드: **ORGN.P-814**

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

POSS Based organic-inorganic hybrid transformer oils

chirumarrysridhar

창원대학교 화학과

Fatty acids and polyols based synthetic esters are suitable environmentally benign alternatives for mineral oil based lubricants and show several applications. In this work a new family of polyhedral oligomeric silsesquioxanes (POSS, which are biodegradable nanostructures with the empirical formula $RSiO1.5$, consists of a rigid and cubic silica core with a 0.53 nm side length surrounded by eight organic corner groups, where R may be a hydrogen atom or an alkyl, alkylene, acryl ate, hydroxyl or epoxide group) based biodegradable oils have been synthesized that bear eight ester functional groups including Type-I and Type-II POSS-Esters from octakis(3-chloropropyl)silsesquioxane (Cl-POSS) and octakis (3-hydroxy propyldi methylsiloxy) octasilsesquioxanes (OHPS), which are alternative to mineral and vegetable oil.

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

Biodegradable hemifluorinated PFOS alternatives: Mono and Bis(sulfonates)

Vijay kumar

창원대학교 화학과

Perfluorooctanesulfonic acid (PFOS) 1 and their derivatives are the key ingredients in many stain repellents and also proven to be toxic towards health and environment due to its non-biodegradability. To reduce the hazardous effects of this perfluoroalkyl chain, we used three partially perfluoroalkyliodides were simultaneously coupled to ethyl vinylsulfonate in presence of Zn/CuI in ionic liquid [BMIM]Cl as well as in formamide to obtain ethylperfluoroalkylsulfonate. Various salts of each sulfonic acid series were synthesized from corresponding ethylsulfonates by hydrolysis.On the other hand we have synthesized the bis sulfonates starting from C4-perfluorianted hydrocarbon. All the compounds are found to be more or less biodegradable and showed good surface tension reduction properties.

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

Synthesis and applications of recoverable mesoporous catalyst Pd-Meso-DBA

Vijay kumar

창원대학교 화학과

Mesoporous silica materials with different textural and structural properties have been synthesized and studied extensively for the past two decades. It has also been successfully demonstrated to act as an excellent heterogeneous catalyst for the broad range of chemical reactions. The key factors for improved catalytic activity are the unique properties such as high surface area, narrowly ordered pore system, high hydrothermal stability and surface functionalities that present inside & outside of pores. So, these heterogeneous mesoporous silica catalyst integrated with all the special properties, can achieve the catalyst-free product with better yield when compared with the conventional catalysts. Thus we present a novel type of mesoporous silica based palladium(0) complex 'Pd-Meso-DBA', and its applications towards Suzuki and Heck coupling reactions.

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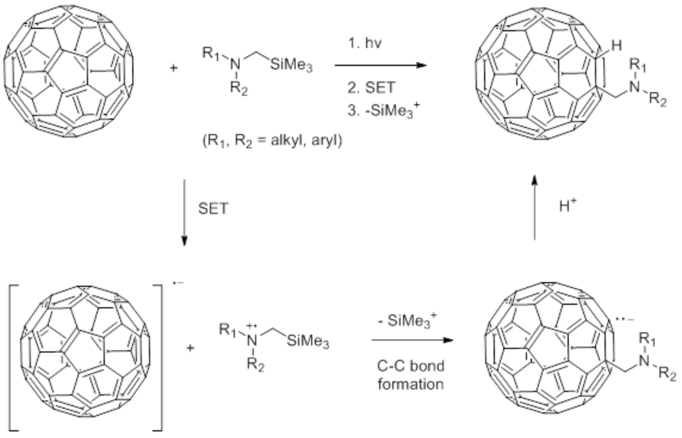
발표분야: 유기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

A Novel Method for the Efficient Synthesis of Functionalized Fullerenes Based on SET Promoted Photoaddition Reactions between alpha-Silylamines and Fullerene C_{60}

임숙현 문경민 이진주 이우솔 조대원*

영남대학교 화학과

Single electron transfer (SET)-promoted photochemical reactions of C_{60} fullerene with alpha-silyl tertiary amines to prepare alpha-aminofullerenes were carried out and their reaction mechanisms were explored. The results showed that photoirradiation of 10% EtOH-toluene solutions containing amine donors and C_{60} fullerene gave rise to formation of alpha-aminofullerenes with modest to high chemical yields. The feasible mechanistic pathways of photoaddition reactions of alpha-silyl tertiary amines with C_{60} leading to the formation of alpha-aminofullerenes described above would begin formation of aminium radical and fullerene anion intermediates arising by SET from alpha-silyl tertiary amines to triplet excited state of C_{60}. Then, EtOH-assisted desilylation from aminium radicals occurs to produce alpha-amino radicals, which form C-C bond with fullerene anion. Finally, subsequent protonation leads to the formation of α-aminofullerenes.


+
R1
N
SiMe3
R2
(R1, R2 = alkyl, aryl)
1. hν
2. SET
3. -SiMe3+
H
R1
N
R2
SET
H+
•−
+
R1
+•
N
SiMe3
R2
- SiMe3+
C-C bond
formation
•−
R1
N
R2

일시: 2014년 4월 16~18일(수~금) 3일간
장소: 일산KINTEX
발표코드: **ORGN.P-818**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthetic Investigation of Trimeric Perylenedimide Containing Benzene as a Core

김성식* T. Majima[1]

전북대학교 화학과 [1]The Institute of Scientific and Industrial Research, Osaka University

Synthesis of trimeric diimides containing perylenediamide and benzene is described. First intermediates were prepared from the corresponding dianhydrides in DMF, imidazole, or pyridine. The chemical yield of the next intermediate, monoimide, was very poor. It was found that 3,5-dinitroaniline was reduced to give triaminobenzene which was use for the next step without isolation. Other types of diimides containing phthalimide, naphthalenediimide and related compounds were also preperaed. Spectroscopic investigation was also discussed.

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장소: 일산KINTEX
발표코드: **ORGN.P-819**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis and Library Construction of Privileged Tetra-Substituted Δ^5-2-Oxopiperazine as β-Turn Structure Mimetics

이원석 박승범[1,*]

서울대학교 생물물리 및 화학생물학과 [1]서울대학교 화학부

In this study, we developed an efficient and practical procedure for the synthesis of tetra-substituted Δ^5-2-oxopiperazine that mimics the bioactive β-turn structural motif of proteins. This synthetic route is robust and modular enough to accommodate 4 different substituents to obtain a high level of molecular diversity without any deterioration in stereochemical enrichment of the natural and unnatural amino acids. Through the in silico studies, including a distance calculation of side chains and a conformational overlapping of our model compound with a native β-turn structure, we successfully demonstrated the conformational similarity of tetra-substituted Δ^5-2-oxopiperazine to the β-turn motif. For the library construction in a high-throughput manner, the fluorous tag technology was adopted with the use of a solution-phase parallel synthesis platform. A 140-membered pilot library of tetra-substituted Δ^5-2-oxopiperazines was achieved with an average purity of 90% without further purification.

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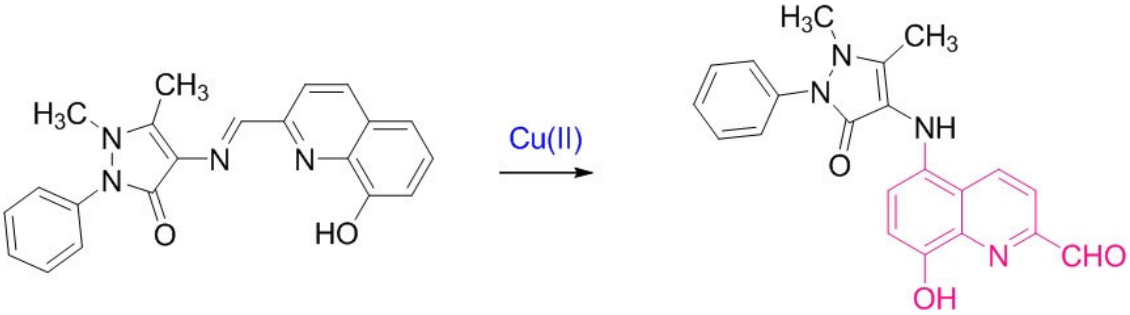
발표코드: **ORGN.P-820**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Reaction-Based Signaling of Cu2+ Ions by a Schiff Base Derived from 8-Hydroxy-2-quinolinecarboxaldehyde

김홍영 김호원 박현지 장석규*

중앙대학교 화학과

Cu(II)-selective signaling behavior of 4-aminoantipyrine appended Schiff base derived from 8-hydroxy-2-quinolinecarboxaldehyde was investigated. The probe revealed Cu(II)-selective chromogenic signaling behavior by the hydrolysis of the enamine moiety followed by oxidative coupling of produced quinolinecarboxaldehyde with 4-aminoantipyrine. Cu(II) selectivity of the signaling was enhanced by displacement approach using in situ generated Hg(II) complex of the probe. Chromogenic Cu(II) signaling in the presence of commonly coexisting metal ions with solution color change from yellow to red was possible with a detection limit of 10^{-7} M.



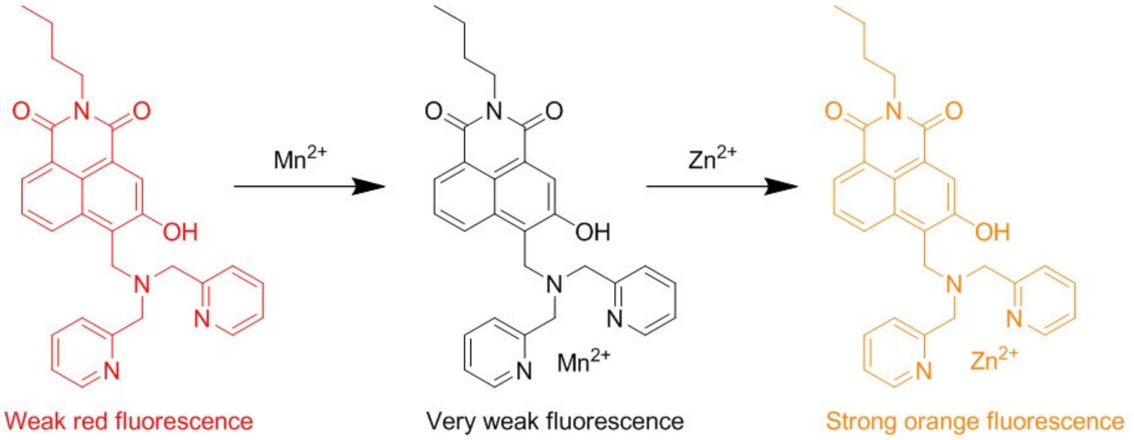
일시: 2014년 4월 16~18일(수~금) 3일간
장소: 일산KINTEX
발표코드: **ORGN.P-821**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Fluorescent signaling of Zn(II) ions by metal ion displacement of Mn(II)-complex of dipicolylamine functionalized hydroxynaphthalimide

이슬기 정용애 최지영 장석규*

중앙대학교 화학과

A new Zn(II)-selective fluorescent signaling probe by metal ion displacement of Mn(II)-DPA(dipicolylamine)-NPIOH(hydroxynaphthalimide) complex was investigated. DPA(dipicolylamine)-NPIOH was prepared by the Mannich reaction of NPIOH with DPA. DPA-NPIOH showed effective quenching with Mn(II) ions. Metal ion displacement of quenched Mn(II) complex of the probe by Zn(II) ions resulted in a prominent fluorescence-on type signaling. Selective Zn(II) ions signaling of the probe was not affected by the presence of commonly encountered metal ions with background. The detection limit for the determination of Zn(II) ions in 99% tris buffered (pH 8.0) aqueous acetonitrile solution was 3.0 x 10^{-7} M. The designed probe could be useful for the visualization of Zn(II) ions in biological samples.



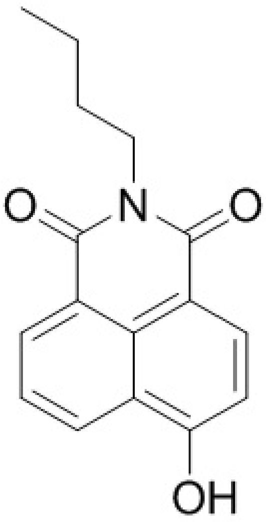
일시: 2014년 4월 16~18일(수~금) 3일간
장소: 일산KINTEX
발표코드: **ORGN.P-822**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Dual signaling of water contents in organic solvents by hydroxynaphthalimides

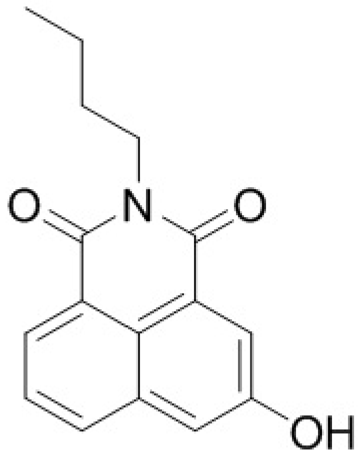
이효진 이슬기 장석규*

중앙대학교 화학과

New fluorescent probes based upon hydroxynaphthalimide(NPI-OH) for the signaling of water content in organic solvents was investigated. Effects of water contents in organic solvents on the hydrogen bonding of NPIOH with water were utilized for the signaling. The probes exhibited chromogenic and fluorogenic signaling behavior in response to the changes in water content in THF, acetonitrile, and DMSO. The changes in fluorescence behavior were successfully analyzed by the ratiometry, and signals well particularly for less than 3% water in the surveyed solvents. The chromogenic and fluorescent behaviors of the NPI-OH system could be used as a convenient probe for the determination of water contents in common organic solvents.



4-NPI-OH



3-NPI-OH

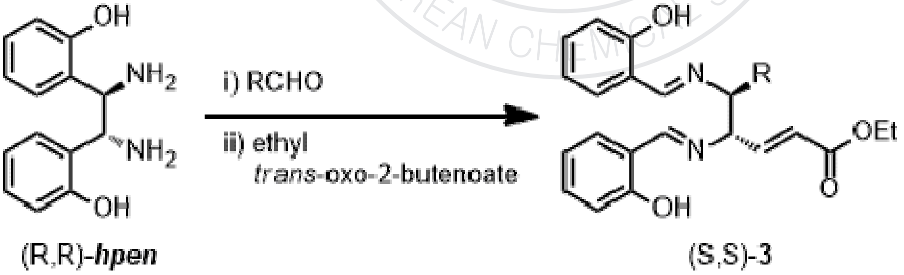
일시: 2014년 4월 16~18일(수~금) 3일간
장소: 일산KINTEX
발표코드: **ORGN.P-823**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Stereospecific Synthesis of γ,δ-Diamino Esters

송명종 김병문*

서울대학교 화학부

γ,δ-Diamino acid structural motifs are commonly found in many bioactive molecules. We report an efficient one-pot reaction for the synthesis of γ,δ-diimino esters with two adjacent chiral centers in enantiomerically pure form through diaza-Cope rearrangement reaction of diimines formed from (R,R)-1,2-bis(2-hydroxyphenyl)-1,2-diaminoethane (hpen) and aldehydes. DFT computation provides interesting insights into the stereospecific rearrangement reaction. The crystal structure of a product diimine formed from the reaction of (R,R)-hpen and 2,6-dichlorobenzaldehyde shows that the reaction gives the product diimine in S,S configuration.



일시: 2014년 4월 16~18일(수~금) 3일간
장소: 일산KINTEX
발표코드: **ORGN.P-824**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Rational Perturbation of the Fluorescence Quantum Yield in Emission-Tunable and Predictable Fluorophores (Seoul-Fluors) by a Facile Synthetic Method Involving CH Activation

최은정 박승범[1,*]

서울대학교 화학과 [1]서울대학교 화학부

Fluorescence imaging enables the uniquely sensitive observation of functional- and molecular-recognition events in living cells. However, only a limited range of biological processes have been subjected to imaging because of the lack of a design strategy and difficulties in the synthesis of biosensors. Herein, we report a facile synthesis of emission-tunable and predictable Seoul-Fluors, 9-aryl-1,2-dihydrolopyrrolo[3,4-b]indolizin-3-ones, with various R1 and R2 substituents by coinage-metal-catalyzed intramolecular 1,3-dipolar cycloaddition and subsequent palladium-mediated CH activation. We also showed that the quantum yields of Seoul-Fluors are controlled by the electronic nature of the substituents, which influences the extent of photoinduced electron transfer. On the basis of this understanding, we demonstrated our design strategy by the development of a Seoul-Fluor-based chemosensor 20 for reactive oxygen species that was not accessible by a previous synthetic route.

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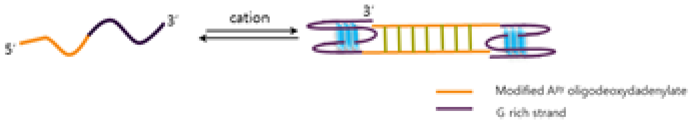
발표분야: 유기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

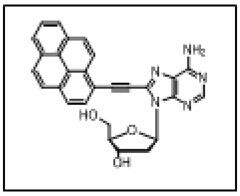
Combination of self-duplex of Apy substituted oligodeoxyadenylate and G-quadruplex

박유진 김병현*

포항공과대학교 화학과

As nucleic acids are able to form well-organized and programmable structure, they are fascinating materials for the construction of nano architectures. Especially, Guanine-rich oligonucleotides are able to form G-quadruplex by stacking G-quartets, in which four guanines are held together by Hoogsteen hydrogen bonding. G-quadruplex has the potential for nano materials because of the artificial design of G-quartets. In addition to, the structures of nucleic acids are stabilized by not only the hydrogen bonding between complementary bases but also the π-π interactions of between nucleobases or nucloebases and intercalators. To generate novel secondary structures, strong π-π stacking interactions in nucleic acids can be used. Previously, my group reported that a covalently linked intercalator induced the structure of a self-assembled homo-deoxyadenylate duplex. In case modified oligodeoxyadenylates featuring ethynyl pyrene-linked 2'-deoxyadenosine (Apy) unsits (inserted in a specific 1,4-relationship) were employed, various ranges of fluorescence emissions were produced as a result of the formation of duplex. Here, the Apy moieties in the oliogodeoxyadenylate provided the fluorescence emissions depending on their numbers.Futhermore, these unique phenomena and structural features have applied to the hybridization of Apy- substituted oligodeoxyadenylate duplex and G-quadruplex, resulting in the construction of high ordered nano materials (Fig. 1). We expect that this concept is applicable the formation of designed nanostructures with regulating properties.

2 



5'- AA^{Py}A AA^{Py}A AA^{Py}A AA^{Py}A GGT TGG TGT GGT TGG

A^{Py}

Fig1. Schemetic illustration of hybridized nanostructure

일시: 2014년 4월 16~18일(수~금) 3일간

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발표코드: **ORGN.P-826**

발표분야: 유기화학

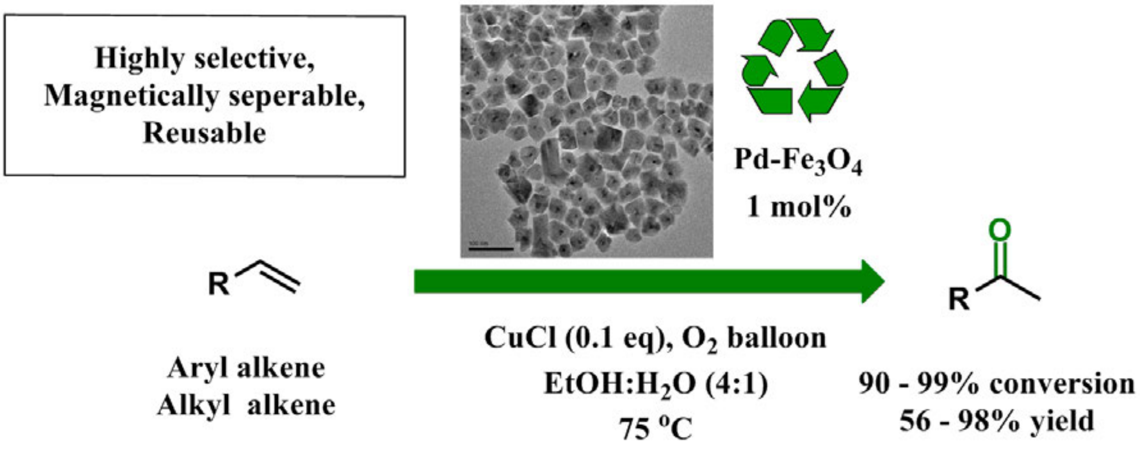
발표종류: 포스터, 발표일시: 수 16:00~19:00

Wacker Oxidation of Terminal Alkenes Using Magnetically Recoverable Pd?Fe3O4 Heterodimer Nanocatalyst

변상문 김병문*

서울대학교 화학부

Wacker oxidation is a useful process for the conversion of a terminal olefin to a ketone.1 We describe herein a new highly selective and environment-friendly Wacker oxidation process employing superparamagnetic Pd?Fe3O4 heterodimer nanocrystals2 as a recyclable catalyst. Various reaction parameters were investigated for the determination of optimal reaction conditions. Consistently high yields and excellent reaction selectivities of the desired Wacker product were observed in almost all the reactions employing the Pd?Fe3O4 nanocrystals in an optimal condition in EtOH-H2O under 1 atm O2.3 This operationally simple oxidation protocol allows recycling of the Pd?Fe3O4 catalyst after the reaction through the use of an external magnet.



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장소: 일산KINTEX
발표코드: **ORGN.P-827**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

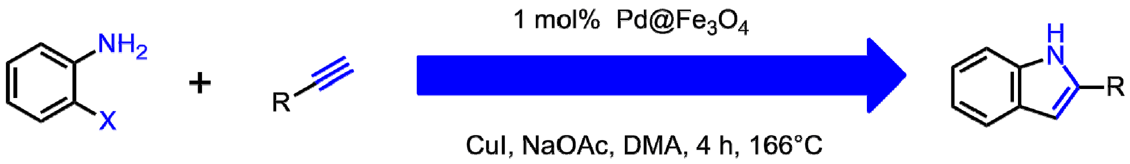
Synthesis of 2-substituted indole derivatives by tandem cyclization using magnetically reusable Pd-Fe_3O_4 nanocrystals

권정민 김병문*

서울대학교 화학부

Indole moiety is found in a wide range of pharmaceutical agents, bulk chemicals, and natural products. So there have been tremendous efforts to synthesize these compounds. However, synthesis of indole is generally carried out in the presence of air sensitive phosphine ligands, phosphine based palladium catalysts or amines, which have characteristic foul smell. Herein, we report the synthesis of 2-substituted indole derivatives under amine- and phosphine-free conditions. Also, using palladium-catalyzed tandem reactions, we could prepare functionalized products with high atom efficiency, circumventing the unwanted waste and saving time and resources. The use of recyclable Pd-Fe_3O_4nanocrystals for the first Songoshira coupling followed by tandem cyclization allowed us to witness successful synthesis of 2-substituted indole derivatives. Pd-Fe_3O_4nanocrystals could be recovered with an external magnet and recycled up to ten times without losing its catalytic activity.

Tandem cyclization



일시: 2014년 4월 16~18일(수~금) 3일간
장소: 일산KINTEX
발표코드: **ORGN.P-828**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Fluorescence modification of the AAAA (4A) loop: toward a probe of the structural transition of the i-motif

박정우 김병현*

포항공과대학교 화학과

The retinoblastoma (RB) gene encodes a tumor suppressor retinoblastoma protein that is dysfunctional in several major cancers. The Rb gene is extremely rich in G and C strands at the 5´ position, potentially forming several secondary structures such as G-quadruplex, i-motif, and Z-DNA species. Among these secondary structures, the i-motif structure is induced by the C-rich strands with hemiprotonated $C{\cdot}C^+$ base pairs under acidic pH. These i-motif sequences are observed repeatedly in eukaryotic genomes. In these regions, several proteins, such as helicase, single strand binding protein, and DNA polymerase, bind specifically to the C-rich strands to regulate the oncogene expression at the transcription level. Thus, the development of new systems for probing structural transition of the i-motif should benefit cancer therapeutics and the study of oncogenes also provides insight into the dynamics of the conformational transitions of C-rich single-stranded DNA as well as complementary G-rich single-stranded DNA.Our goal is to develop a simple and efficient fluorescence signaling system for probing the structural transition of i-motif of Rb gene from single strand and duplex forms to i-motif structures. The Rb gene sequence has the AAAA (4A) loop region on which we focused to induce variations in observable signals representing conformational transition from single-stranded and duplex forms to the i-motif structure without disturbing the hemiprotonated $C{\cdot}C^+$ base pairs at low pH. Pyrene-modified deoxyadenosine (^{Py}A) is used as a fluorophore unit, which is sensitive to its local environment and can be incorporated into several DNA structures. Various oligodeoxynucleotides were synthesized to systematically probe the structural transitions of the i-motif, incorporated pyrene units at the 1 (ODN i1), 1,2 (ODN i2), 1,3 (ODN i3), and 1,4 (ODN i4) positions of the 4A loop. Ready modification with the structurally simple fluorophore ^{Py}A provides sequences that do not require any additional quencher for fluorescence detection. In terms of fluorescence signals, ODN i2 and ODN i4, two ^{Py}A units incorporated at the 1,2 positions and

1,4 positions of the 4A loop respectively, provide the most dramatic fluorescence changes excitation wavelength upon the conformational transitions. In addition, we observed that the conformational transitions of all the modified ODNs from i-motif to single strand were not simple one-stage transitions.

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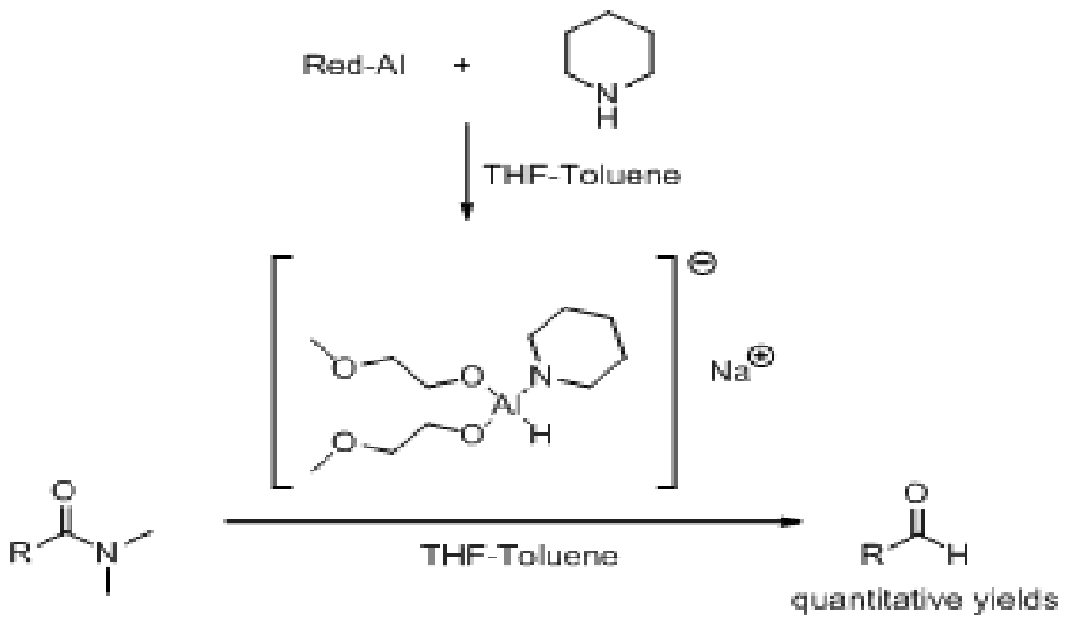
발표분야: 유기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Effective Synthetic Method of Aldehydes from Tertiary Amides Using New Modified Red-Al Reducing Agent

장희망 최병훈 신원규 강대훈 안덕근*

강원대학교 화학과

Aldehydes are valuable building blocks and reactive intermediates in organic synthesis. The general and classical syntheses of aldehydes from carboxylic acid derivatives involve reduction-oxidation and partial reduction using efficient partial reducing agents. Obviously, one-step partial reduction methods are more useful than two-step reduction-oxidation methods owing to their simplicity, and generality in organic synthesis. We very recently found a very effective and new modified Red-Al (sodium bis[2-methoxyethoxy]aluminum hydride) reducing agent that was easily prepared by reacting commercially available Red-Al with piperidine for the synthesis of aldehydes from tertiary amides in quantitative yields. Red-Al derivatives of secondary amines such as morpholine, N-methylpiperazine, or pyrrolidine can be used for the partial reduction of esters or diesters. However, there is not reported that general partial reducing methods of tertiary amides to aldehydes using modified Red-Al reducing agent including Red-Al.


Red-Al
+
THF-Toluene
Na
Al
THF-Toluene
quantitative yields

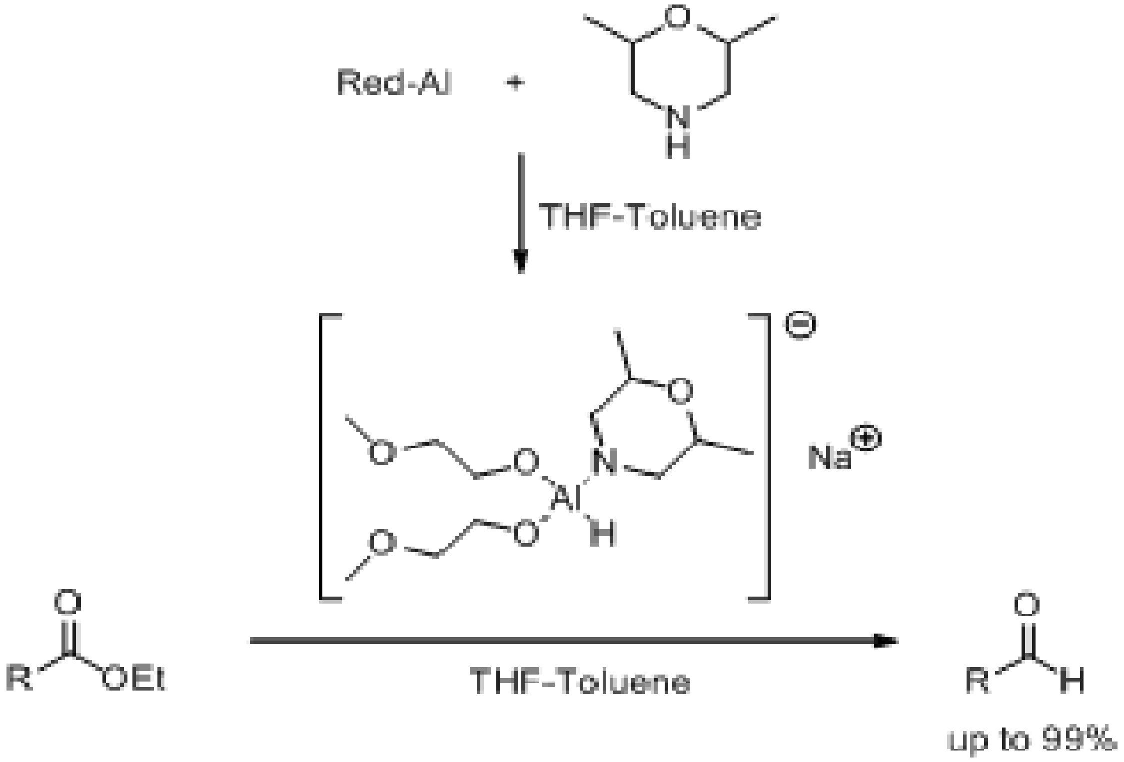
일시: 2014년 4월 16~18일(수~금) 3일간
장소: 일산KINTEX
발표코드: **ORGN.P-830**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Partial Reduction of Esters to Aldehydes Using a Novel Modified Red-Al Reducing Agent

신원규 강대훈 안덕근*

강원대학교 화학과

We have developed a convenient alternative method for the synthesis of aldehydes from both aromatic and aliphatic esters in very good to excellent yields in the absence of any additives using a modified Red-Al that was easily prepared by reacting commercially available Red-Al with cis-2,6-dimethyl morpholine. The advantages of the present methodology are as follows: (i) simple preparation procedure of the reducing agent, (ii) improved product yields, (iii) convenient reaction temperature, and (iv) short reaction times. Therefore, the new reagent has great potential to be a useful alternative partial reducing agent for the synthesis of aldehydes from esters in organic synthesis.


Red-Al
+
THF-Toluene
Na
THF-Toluene
up to 99%

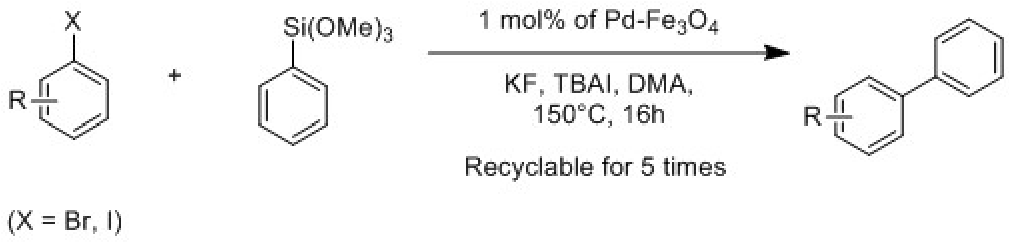
일시: 2014년 4월 16~18일(수~금) 3일간
장소: 일산KINTEX
발표코드: **ORGN.P-831**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Ligand-free Hiyama cross-coupling reactions with magnetic Pd-Fe_3O_4 heterodimer nanocrystals as a recoverable catalyst

이웅섭 변상문 권정민 김병문*

서울대학교 화학부

Hiyama cross-coupling reaction is considered as a meritorious alternative producing biaryl derivatives using inexpensive, environmentally benign and readily available organosilicon reagents.[1] Herein we report ligand-free Hiyama cross-coupling reactions using superparamagnetic Pd-Fe_3O_4 heterodimer nanocrystals[2] (1 mol% in Pd) as a recyclable catalyst. The nanocrystal catalysts exhibited good activities, accommodating a fairly wide range of substrates including aryl bromides and iodides with varying steric and electronic properties. Furthermore, the nanocrystal catalyst could be easily recovered using an external magnet and recycled five times without losing its catalytic activity to a considerable degree.References1. (a) Hiyama, T., *J. Organomet. Chem* 2002, 653, 58. (b) Denmark, S. E.; Sweis, R. F., *Acc. Chem. Res* 2002, 35, 835.2. (a) Jang, Y.; Kim, S.; Jun, S. W.; Kim, B. H.; Hwang, S.; Song, I. K.; Kim, B. M.; Hyeon, T., *Chem Commun*, 2011, 47, 3601. (b) Chung, J.; Kim, J.; Jang, Y.; Byun, S.; Hyeon, T.; Kim, B. M., *Tetrahedron Lett* 2013, 54, 5192.



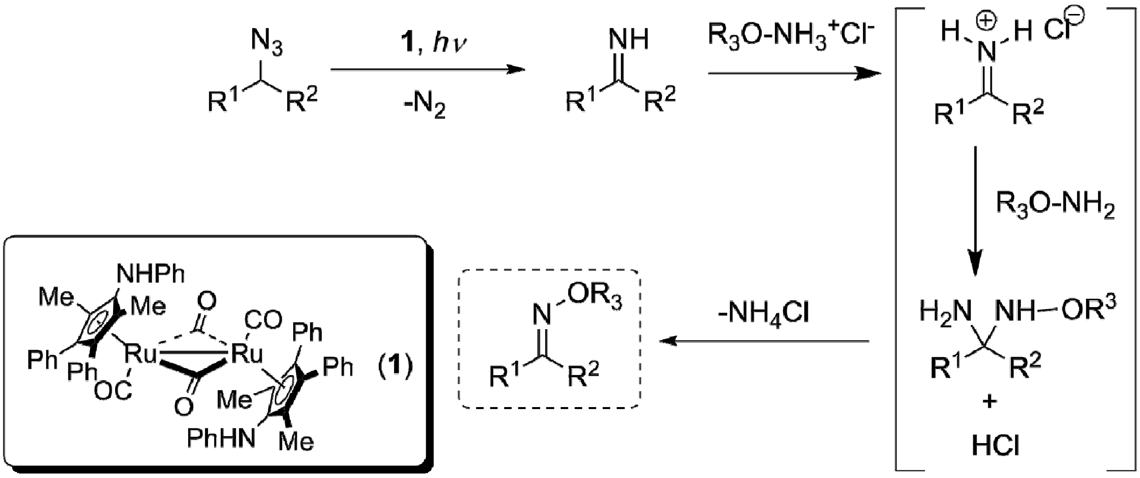
일시: 2014년 4월 16~18일(수~금) 3일간
장소: 일산KINTEX
발표코드: **ORGN.P-832**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Ru-catalyzed transformation of alkyl azides into O-alkyl oximes by one-pot imine formation/nucleophilic substitution squence

전미나 박재욱[1,*]

포항공과대학교 화학 [1]포항공과대학교 화학과

O-alkyl oxime has been recognized as an important functional group which is frequently found in numerous bioactive compounds such as fluvoxamine, oxiconazole, roxithromycin. O-alkyl oximes are also used as important reagents for various organic transformations such as synthesis of amino acids, asymmetric reduction into chiral amines, C-H bond activation reactions. We developed a new protocol for O-alkyl oxime synthesis from various azide precursors; N-unsubstituted imines generated from azides by Ru-catalysis are utilized by the tandem condensation reaction with numerous O-alkylhydroxylamine salts. This is the notable demonstration of the applicability of N-unsubstituted imines, showing a clear advantage in terms of mild reaction conditions and chemoselectivity. In the reaction, N2 and NH3 are the only by-products, where in-situ generated NH3 capture the excess acid which eliminates the requirement of use of external additives added an extra advantage.



일시: 2014년 4월 16~18일(수~금) 3일간
장소: 일산KINTEX
발표코드: **ORGN.P-833**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Fluorescent nucleic acid probes for the G-quadruplex-forming sequences

김기태 이하정 김병현*

포항공과대학교 화학과

G-rich sequences containing series of GGG bases are prevalent in telomeric DNA and oncogene promoter regions to form G-quadruplex frequently involved in a variety of genetically important phenomena. Due to the importance of the G-quadruplex in the biological systems, there has been a demand for developing efficient fluorescent probes for detection and visualization of G-quadruplex-forming sequences to understand G-quadruplexes. Herein, we introduced two synthesized nucleosides, ^{Bod}U and ^{DNS}C. ^{Bod}U were synthesized by Sonogashira coupling reaction between a 5-iodo-2´-deoxyuridine and ethynyl-BODIPY. Dansyl group was chemically attached to N4 position of 2´-deoxycytidine to give ^{DNS}C. Using these two nucleosides, we designed two different types of fluorescent nucleic acid systems for probing the G-quadruplex-forming sequences based on competition between two interstrand G-quadruplexes containing ^{Bod}U and direct detection of GGG triad sequence by ^{DNS}C.References1. Wright W. E., Tesmer V. M., Huffman K. E., Levene S. D., Shay J. W., *Genes Dev.* 1997, *11*, 2801.2. Brooks T. A., Kendrick S., Hurley L., *FEBS J.* 2010, *277*, 3459.3. Kim K. T., Kim B. H., *Chem. Commun.* 2013, *49*, 1717.4. Kim K. T., Kim H. W., Moon D. H., Rhee Y. M., Kim B. H., *Org. Biomol. Chem.* 2013, *11*, 5605.

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발표코드: **ORGN.P-834**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

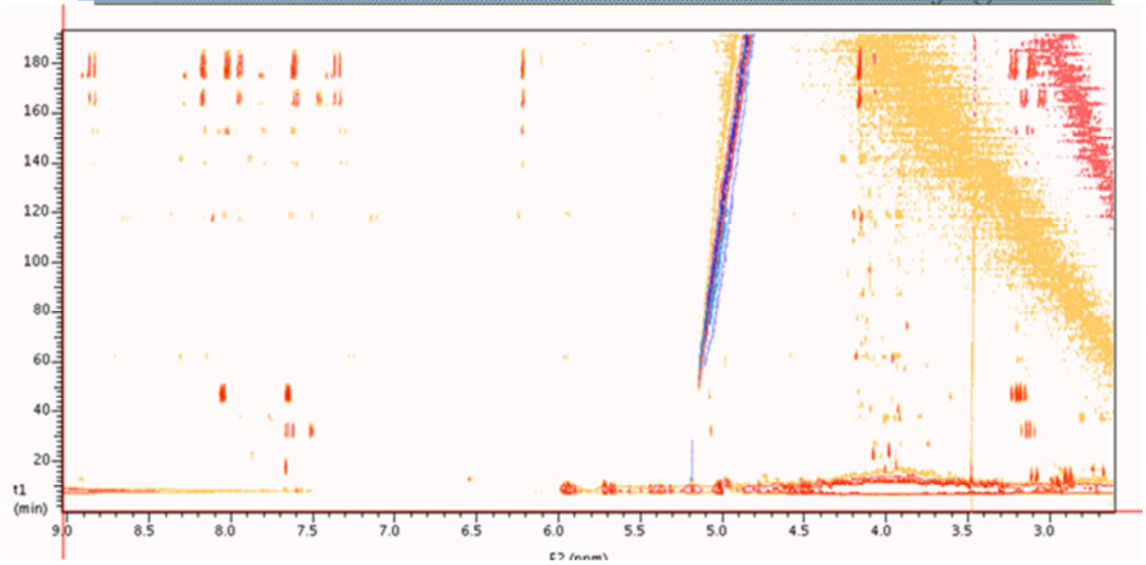
Structural Elucidation of Phenolic Compounds in Natural Product Extracts by LC-NMR

이영주* 이기복[1]

한국기초과학지원연구원 광주센터 [1]전남대학교 화학과

The coupling of LC (liquid chromatography) with NMR (nuclear magnetic resonance) spectroscopy is used as a powerful analytical tool, which rapid structural screening is possible without tedious and time-consuming isolation step. With online LC-NMR spectroscopic analysis a mixture of chemical compounds is injected onto a HPLC column and the separated components are directly analyzed online with NMR spectrometer using a flow probe. Due to the intrinsically low sensitivity of NMR spectroscopy, proton, the most sensitive nuclei in natural abundance, is generally selected for online LC-NMR detection. Here we optimized LC-NMR experiments, which is helpful to elucidate the structure of bioactive compounds from n-BuOH extracts of Cimicifuga Heracleofolia rhizomes extracts exhibiting cytotoxicity against colon cancer cells (HCT-116). The 1H NMR spectra of the BuOH extracts were run in the onflow mode and each of 8 compounds was identified as cimicifugic acid A, B, E, F, shomaside B, fukiic aicd, ferulic acid, and pisicidic acid. An additional ROESY1D spectrum measured for the peak 4 confirmed the structure of cimicifugic acid F. The rapid structural analysis of both major and minor components of this class of compounds demonstrated the power of structure-guided screening as a complementary method to assay-guided screening.

Onflow LC-NMR on BuOH extract of *Cimicifuga.H*



일시: 2014년 4월 16~18일(수~금) 3일간
장소: 일산KINTEX
발표코드: **ORGN.P-835**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Fluorescent Oligonucleotide Probe for Huntington’s disease Detection

노종진 김병현*

포항공과대학교 화학과

In the early 1990’s, a new class of molecular disease, TNR disease, has been characterized, arising from unstable and abnormal expansions of DNA-trinucleotides. These disorders affect gene expression. If the repeat of DNA-trinucleotide is present in a healthy gene, dynamic mutation may increase the repeat count and result in a defective gene. Of these, CAG repeats are translated into a series of uninterrupted glutamine residues which is known as a poly-glutamine (poly Q). It may be subject to increased aggregation and affects all mammalian cells. This disorder as the Huntington’s disease symptom can begin at any age from infancy to old age. Through genetic anticipation, the disease might develop earlier in life in each successive generation. We can use various molecular beacon systems with fluorophore for the rapid detection of the Huntington’s disease.We prepared a modified CTG repeat detector with fluorophore and quencher as such a molecular beacon structure. If it exists alone in solution, it makes a molecular beacon structure with no fluorescent signal. But if it exists with CAG repeat targets, it can make duplex with targeted units by complementary DNA pairing, which can show strong fluorescent signal. In our designed model system, the fluorescence intensity is enhanced by more than 10 folds upon the hybridization with a perfectly matched target oligonucleotide.

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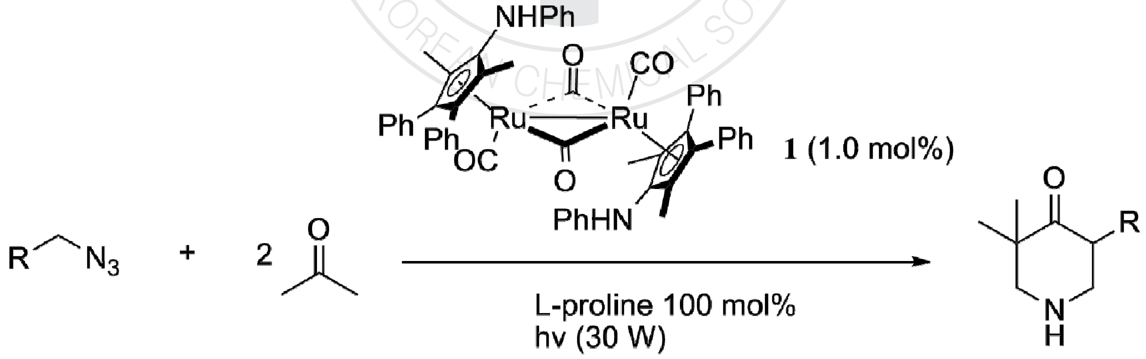
발표분야: 유기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

The construction of 2,2-dimethyl-6-substituted 4-piperidones by tandem-Mannich reaction of N-unsubstituted imines

한정훈 이영호* 박재욱*

포항공과대학교 화학과

We deveolped a one-pot and simple synthetic method of 2,2,6-trisubstituted 4-piperidones from alkyl azide, acetone and L-proline under mild conditions: N-unsubstitued imines are generated from alkyl azides by a photo-activated ruthenium catalyst, followed by tandem-Mannich reaction. This transformation showed good chemoselectivity and wide substrate scope. Now, study of asymmetric transformation is on going in our laboratory.



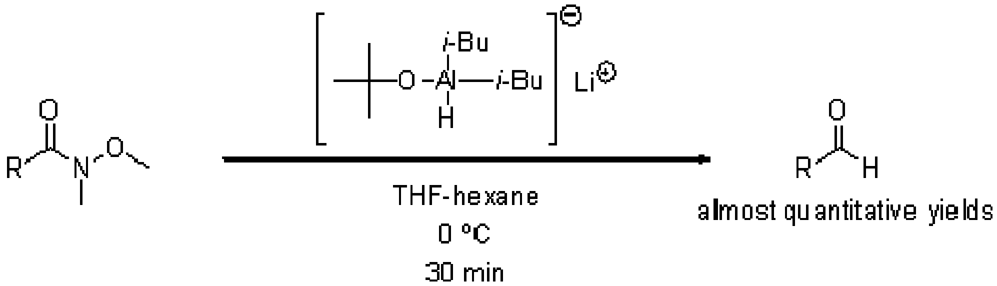
일시: 2014년 4월 16~18일(수~금) 3일간
장소: 일산KINTEX
발표코드: **ORGN.P-837**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Application of LDBBA (Lithium diisobutyl-t-butoxyaluminum hydride) for synthesis of aldehydes form Weinreb amides

안재성 장희망 김예슬 진실아 안덕근*

강원대학교 화학과

Weinreb amides are recognized as reliable intermediates for the preparation of aldehydes and ketones from carboxylic acid derivatives, and their synthetic utility has been widely demonstrated in organic synthetic fields. However, the yields of the desired aldehydes from the reactions involving Weinreb amides are fairly low (67～76%) even at -78 °C using DIBALH or LiAlH4 generally. Recently, we reported already that LDBBA had valuable ability as partial reducing agent and commercially available from Aldrich Chemical Company now. Fortunately, we found that LDBBA was also very effective partial reducing agent for the synthesis of aldehydes from Weinreb amides in almost quantitative yields at mild reaction temperature (0 °C).



일시: 2014년 4월 16~18일(수~금) 3일간
장소: 일산KINTEX
발표코드: **ORGN.P-838**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Efficient synthesis of secondary Amides using trimethyl aluminum reagent

정성수 이상협*

대구가톨릭대학교 생명화학과

We researched highly effective reaction of Amides from a trimethyl aluminum reagent, with several kinds of Alkynes. We choose and tested alkyl, aryl, and some sorts of specific isocyanates which has different functional groups. Starting with isocyanate, to conform secondary Amides is moderate, reaction is going under mild conditions and reaction time is less than 30 minutes. All the desire product is conformed with reliable yield, and there are not much amount of side-product.We expect, theses stabilized secondary Amides are great part of reaction which is using trimethyl aluminum reagent, and also it is meaningful to make Amides from several Isocyanates.

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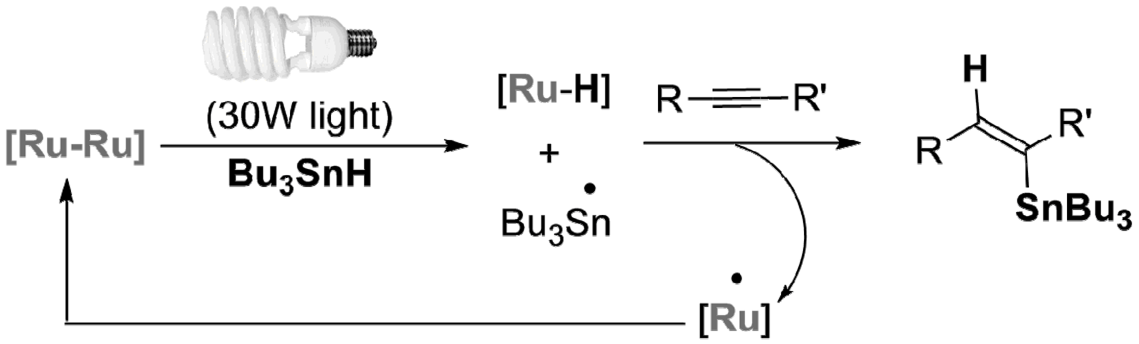
장소: 일산KINTEX
발표코드: **ORGN.P-839**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Novel Ruthenium Photocatalyst for Highly Regio- and Stereoselctive Hydrostannation of Alkynes at Room Temperature

Gupta Sreya 이영호* 박재욱*

포항공과대학교 화학과

Organostannanes are valuable intermediates in organic synthesis due to their versatility in C-C bond forming reactions. There are many methods for preparing vinylstannanes, among them the direct addition of tin-hydride to alkyne (hydrostannation) is the most attractive one in the view of efficiency and atom-economy. Numerous catalyst system based on transition metal-catalyzed syn-stereoselctive and radical initiator mediated anti-stereoslective hydrostannation has been developed, however controlling regio- and stereoselctivity are remained as a challenging task in the field of organic synthesis. Herein a novel catalyst system has developed for the hydrostannation of a range of alkynes with tributylstannane under mild conditions. The active catalytic species was formed from a stable dinucler complex under household fluoresecnt light (30 W) at room temperature. This ruthenium-catalyzed hydrostannation has shown a remarkable regio- and stereoselctivity for various internal and terminal alkynes. The regio- and stereoselectivity for the vinylstannanes resemble to those in radical-mediated hydrostannation, but has clear advantages in reaction efficiency over conventional ones using AIBN and BEt3, including the recyclability of the ruthenium catalyst.



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장소: 일산KINTEX
발표코드: **ORGN.P-840**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Application of Organoaluminum reagents in the Synthesis of Amidines and α,β-Alkynyl Ketones

BALAJI 이상협[1,*]

대구가톨릭대학교 화학과 [1]대구가톨릭대학교 생명화학과

So far, many organoaluminum reagents have proven as remarkable reagents in organic synthesis due to their inherent reactivity, wide range of applicability, low cost and commercial availability. Organoaluminum compounds can easily react with various heteroatoms in organic molecules, particularly with oxygen and nitrogen, even with carbon to form a strong coordinate complex (1:1). One widely used reagent of note is dimethylaluminum amide, derived from the reaction between trimethylaluminum and coerresponding amine. This reagent has been utilized in the direct conversion of ester or acid to amide, carbamate to urea. As a latter example, Micouin et al. developed the alkynyldimethylaluminum reagent from the reaction of alkynes with trimethylaluminum using a catalytic amount of Et3N. This reagent has been utilized in a wide range of organic transformations, such as alkynylative ring opening of activated epoxides or oxazolidines, Pd-catalyzed cross-coupling reaction and in the synthesis of aluminoisoxazoles, and pyrazoles, etc

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발표코드: **ORGN.P-841**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis of 3-amino-1-quinoxalin-2(1H)-one library, 4- preliminart solution-phase test

RAMACHANDRAN 이상협[1,*]

대구가톨릭대학교 화학과 [1]대구가톨릭대학교 생명화학과

Combinatorial solid-phase organic synthesis (SPOS) provides the main driving force for the preparation of small organic molecules libraries for application in lead discovery and high-throughput medicinal chemistry research within the pharmaceutical industry. Our research program has focused on the application of polymer-bound α-diazo-β-ketoesters as key building blocks for the diversity-oriented synthesis of a series of a nitrogen-containing heterocyclic compound libraries, including oxazoles, indoles, imidazolones, pyrazines and pyrazines, etc.Initially, ethyl 2-(2-azidophenylamino)-2-oxoacetate, which was previously obtained from the coupling reaction between ethyl 2-chloro-2-oxoacetate and azidoaniline was subjected to N-alkylation with various alkylating agents in presence of LiHMDS. Then, these alkylated products were cyclized by the treatment of TPP to yield corresponding 3-amino-1-quinoxalin-2 (1H)-ones via Staudinger reaction followed by aza-Wittig reaction, which can be finally derivatized by Lewis acid mediated smart cleavage.

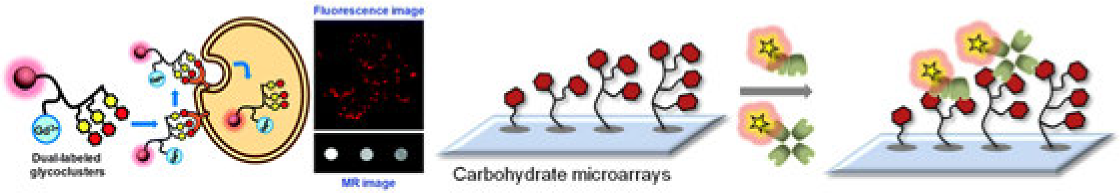
일시: 2014년 4월 16~18일(수~금) 3일간
장소: 일산KINTEX
발표코드: **ORGN.P-842**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis of glycocluster synthesis for studies of functional glycomics

배재영 신인재*

연세대학교 화학과

Glycans, which are found mainly in the form of glycoconjugates such as glycoproteins, proteoglycans, and glycolipids inside or on the surface of cells, participate in a wide range of physiological and pathological processes through interactions with proteins. It is generally accepted that multivalent interactions between glycans and proteins enhance an otherwise weak binding affinity of monomeric sugars with receptors. Enhancements in binding affinity by multivalent interactions (often referred to as the cluster glycoside effect) are attributed to the chelate effect, clustering of carbohydrate-binding proteins, or statistical rebinding. To readily obtain glycoclusters with diverse spatial separation and various valences of sugars, we have developed an efficient solid-phase synthetic strategy for peptide-based glycoclusters. By using this methodology, various glycoclusters with a valence ranging from 1 to 4 and different spatial arrangements of the sugar ligands were prepared. And we used these glycoclusters for studies of functional glycomics.



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장소: 일산KINTEX
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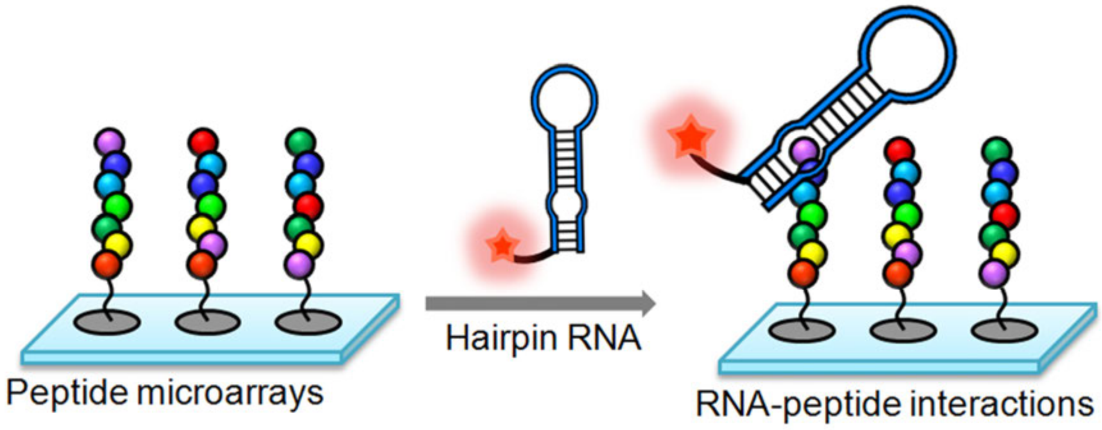
발표분야: 유기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Peptide microarrays as a powerful tool for rapid profiling of RNA-peptide interactions

배재영 신인재*

연세대학교 화학과

A rapid and quantitative method to evaluate binding properties of hairpin RNAs to peptides using peptide microarrays has been developed. The microarray technology was shown to be a powerful tool for high-throughput analysis of RNA?peptide interactions by its application to profiling interactions between 111 peptides and six hairpin RNAs. The peptide microarrays were also employed to measure hundreds of dissociation constants (Kd) of RNA?peptide complexes. Our results reveal that both hydrophobic and hydrophilic faces of amphiphilic peptides are likely involved in interactions with RNAs. Furthermore, these results also show that most of the tested peptides bind hairpin RNAs with submicromolar Kd values. One of the peptides identified by using this method was found to have good inhibitory activity against TAR?Tat interactions in cells. Because of their great applicability to evaluation of nearly all types of RNA?peptide interactions, peptide microarrays are expected to serve as robust tools for rapid assessment of peptide?RNA interactions and development of peptide ligands against RNA targets.



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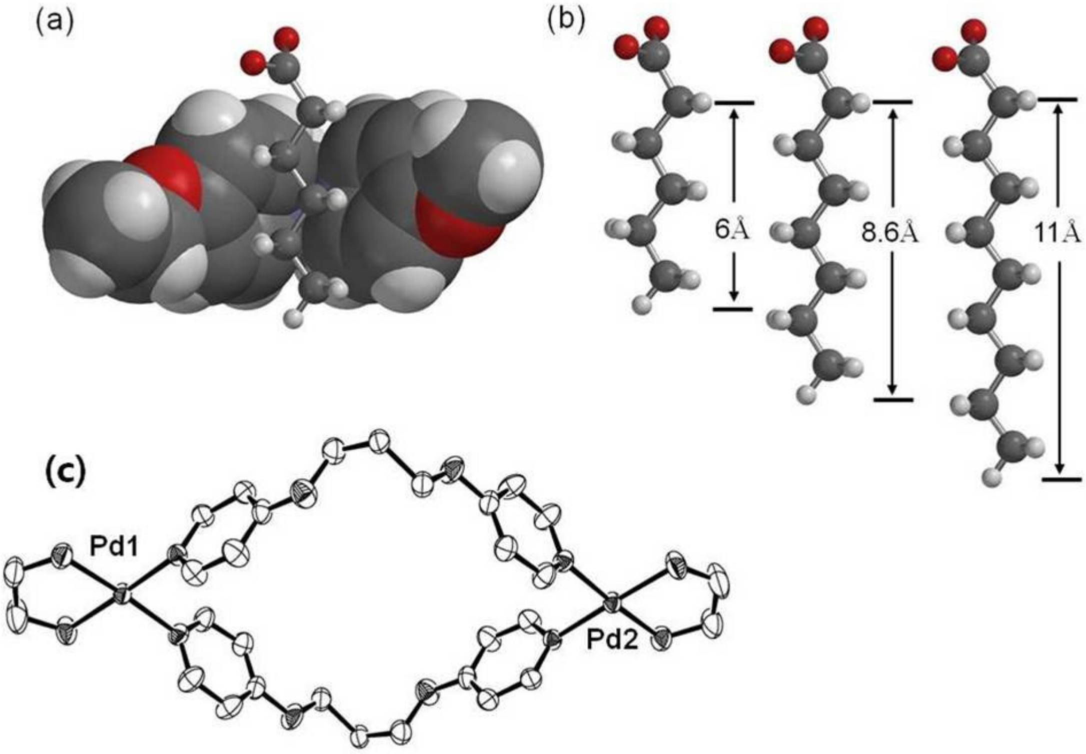
장소: 일산KINTEX
발표코드: **ORGN.P-844**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Fatty Acid Binding Study of Pd (II) Self-Assembled Macrocycle

송영란 천지현 임춘우[1,*] 김태우[*]

경희대학교 동서의학대학원 [1]한남대학교 화학과

The dynamic behavior of fatty acids in the hydrophobic cavity of a macrocycle was investigated. Helical coiling of two fatty acids was compared through NMR titration experiments. As a further study, we measured the binding constants between the PdII self-assembled macrocycle and various fatty derivatives using NMR titration or isothermal titration calorimetry. The guests have different lengths (C4 to C8) or are partially/fully fluororated. In addition we confirmed the solid state structure of the PdII self-assembled macrocycle by X-ray crystallography after counteranion-exchanging from NO2- to PF6-. The Solid state structure matches well with NMR interpretation and Gaussian calculation.


(a)
(b)
6Å
8.6Å
11Å
(c)
Pd1
Pd2

일시: 2014년 4월 16~18일(수~금) 3일간

장소: 일산KINTEX

발표코드: **ORGN.P-845**

발표분야: 유기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

[발표취소] E-beam Mediated Ligand Dissociation of Diyne-Dicobaltcarbonyl Complexes as Potential Photochemical Alkyne Precursor

최정철 황광진[1,*]

홍익대학교 화학시스템공학과 [1]홍익대학교 바이오화학공학과

발 표 취 소

본 논문은 발표취소된 논문입니다.

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Design, Synthesis and in-vitro Screening of Potential ROS1 Kinase Inhibitors having 4-(2-phenyl)pyridin-4-yl 1H-Pyrazole scaffold and its isoxazole analogues

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One of the most promising targets for the rational design of anti-cancer drugs is the ROS receptor tyrosine kinase as its molecular alterations has been recently shown its implication in non-small cell lung cancer (NSCLC). Therefore, a new series of 12 compounds; 6 compounds sharing 4-(2-(4-substitutedphenyl)pyridin-4-yl)-3-(3-methoxy-5-methylphenyl)-1H-pyrazoles scaffold (4a-f) and the other 6 compounds having isoxazole analogues (5a-f) has been rationally designed, synthesized and screened against ROS1 kinase to be a potential agent for treatment of NSCLC. Compounds 4b, 4c and 4e showed moderate inhibitions against ROS kinase. Compound 4e has showed the strongest inhibitions with IC50 values of 1.25 μM against ROS kinase. A brief structure-activity relationship study and a molecular modeling study were made revealing a group of essential structural features for good kinase inhibitory activity within this new class of kinase inhibitors.

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발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis and biological evaluation of new pyrazol-4-ylpyrimidine derivatives as potential and selective inhibitors for ROS1 kinase

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With the aim of discovering potent and selective kinase inhibitors targeting ROS1 kinase, we have designed, synthesized and screened a series of new pyrazol-4-ylpyrimidine derivatives based on our previously discovered lead compound KIST301072. Compounds (6a-e and 7a-e) showed good to excellent activities against ROS1 kinase, and seven out of the ten tested compounds were more potent than KIST301072. Also compound 7c was the most potent, with IC50 of 24 nM - around two times more potent than Crizotinib against ROS1 kinase. Moreover, compound 7c showed ROS1 inhibitory selectivityof about 170-folds, relative to that of ALK sharing about 49% amino acid sequence homology with ROS1kinase in the kinase domain

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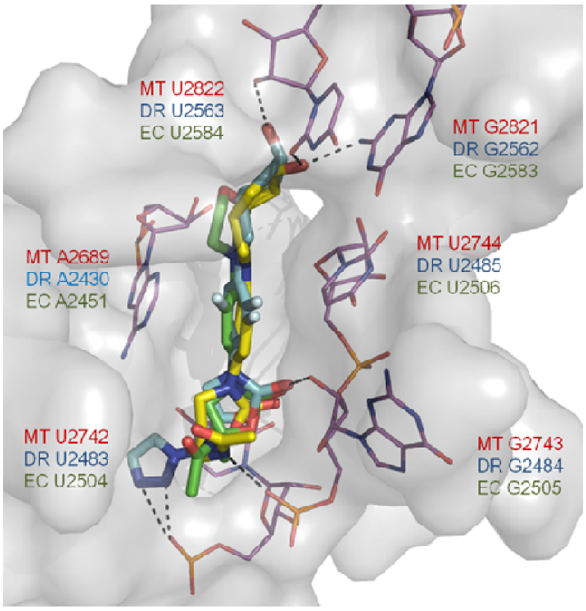
발표종류: 포스터, 발표일시: 수 16:00~19:00

Novel Azabicyclic Oxazolidinone Antibacterials; Synthesis, Biological Evaluation, and Docking Studies against resistant strains

이주현 서선희[1] 강순방[1] 배애님[2] 정낙철 금교창[3,*]

고려대학교 화학과 [1]한국과학기술연구원(KIST) 뇌의약연구단 [2]한국과학기술연구원(KIST) 생체과학연구본부 [3]한국과학기술연구원(KIST) 케모인포메틱스연구센터

Linezolid is the first approved oxazolidinone class antibacterial, which inhibits bacterial protein synthesis at the peptidyltransferase center (PTC) in 50S ribosomal subunits. Linezolid demonstrates potent antibacterial activities against resistant strain such as methicillin-resistant Staphylococcus aureus (MRSA) and vancomycin-resistant Streptococcus pneumoniae. However, oxazolidinone-resistant strains of MRSA and VREF emerged in the clinics. Development of new oxazolidinone classes showing high potency against linezolid-resistant strains has been extremely studied.We synthesized novel azabicyclic oxazolidinone series having extended C-ring and C-5 side chain of the oxazolidinone A-ring, and evaluated their antimicrobial activities against Mycobacterium tuberculosis, Gram-positive, and Gram-negative resistant strains. Several compounds showed good in vitro antimicrobial activities. Especially, endo-alcohol 2a and exo-alcohol 2b displayed four fold higher activities than linezolid against M. tuberculosis H37Rv.Furthermore, the molecular docking studies of endo-alcohol 2a and exo-alcohol 2b were accomplished at the PTC in 50S ribosomal subunits of Deinococcus radiodurans. The two compounds demonstrated good total scores and Cscores compaired with linezolid. The docking results were well correlated with in vitro assay data.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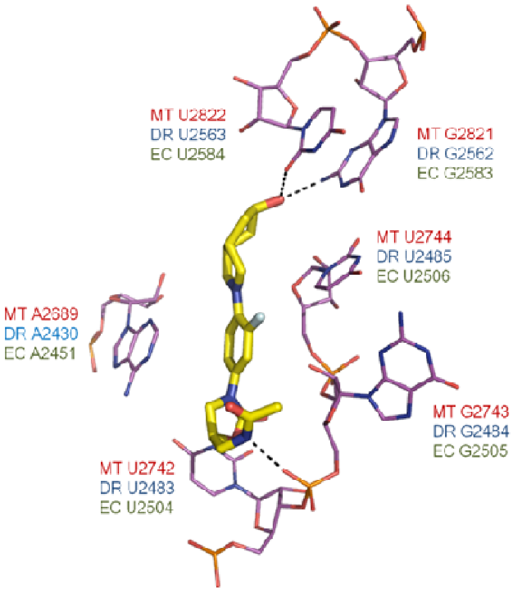
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MT G2743
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EC G2505
MT U2742
DR U2483
EC U2504

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발표종류: 포스터, 발표일시: 수 16:00~19:00

Novel 2-Aminopurine Derivatives as Hsp90 Inhibitors; Synthesis, X-ray Crystallographic Studies and Biological Evaluation for Anticancer agents

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Heat-shock protein 90 (Hsp90), an ATPase-dependent protein folding molecular chaperone, regulates the stability and function of many client proteins such as Src, cdk4, Akt, HER2/neu, EGFR, c-Kit, and Raf-1. Many of misfolded client proteins play critical roles in cancer progression. Hence, inhibition of Hsp90 leads to destabilize the client proteins by conformational change of between Hsp90 and client proteins. And then, these oncogenic client proteins undergo degradation via ubiquitin-dependent pathway. Development of Hsp90 inhibitors has been extensively studied as a target of cancer therapy. Among Hsp90 inhibitors, we are interested in the purine based inhibitors such as CUDC-305, PU-H71, MPC-3100, and BIIB021.Herein, a series of 2-aminopurine derivatives were synthesized, and evaluated against SKBR3, MCF-7, and HCT116 cancer cell lines. Several compounds displayed good anti-proliferative activities in in vitro assay, and also showed high binding affinity for N-terminal Hsp90α in ITC and FP competition assay. Among them, KKK5142 showed highest binding affinity similar to BIIB021 in FP competition assay. Moreover, X-ray crystallographic data of KKK5142-Hsp90 complex demonstrated that KKK5142 bound in the N-terminal ATP-binding domain with stable binding conformation. The ring substituents at N-7 position displayed hydrophobic interaction with Leu107, and aryl ring at N-9 position exhibited π-π stacking interaction with Phe138 in the hydrophobic pocket by reserving the conformation of outer helix.

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발표종류: 포스터, 발표일시: 수 16:00~19:00

Broad-Spectrum Anticancer Diarylureas and Diarylamides Possessing Pyrrolo[2,3-d]pyrimidine Scaffold

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A series of diarylureas and diarylamides possessing pyrrolo[2,3-d]pyrimidine scaffold was designed and synthesized. The in vitro antiproliferative activities of a selected group of the target compounds against NCI-60 cell line panel were tested and compared with Sorafenib and Imatinib as reference compounds. Most of the compounds showed strong and broad-spectrum antiproliferative activities. Compounds IVa, IVb, and IVd with benzamido moiety at position 4 of the pyrrolo[2,3-d]pyrimidine nucleus, para-disubstituted phenyl ring at N1-position of pyrrolo[2,3-d]pyrimidine scaffold, and urea linker showed strong and broad-spectrum anticancer results with high potencies and efficacies. In addition, the amide derivatives Vb and Vc demonstrated one-digit nanomolar IC50 values over two and one cell line(s), respectively. Amid all the target compounds, compound IVa demonstrated the best results in both one-dose and five-dose testing modes. It showed 109.18% mean % inhibition over the NCI-60 cancer cell line panel at 10 μM concentration, submicromolar IC50 values over eight cell lines of eight different cancer types, and high efficacy with total growth inhibition (TGI) and 50% lethal concentration (LC50) values less than 4.22 μM over three colon, ovarian, and prostate cancer cell lines. It showed superior potency and efficacy to Sorafenib and Imatinib over most of the tested cell lines.

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발표종류: 포스터, 발표일시: 수 16:00~19:00

Design, synthesis and biological evaluation of novel diarylamide derivatives possessing 1,3,4-oxadiazole as potential anticancer agents

Mahmoud Gamal Eldin* **Mohammed I. El-Gamal[1,*]** **Mohammed Samir*** **오창현[2,*]**

과학기술연합대학원대학교(UST) Biomolecular science [1]한국과학기술연구원(KIST) 생체재료연구단, Department of Medicinal Chemistry, Faculty of Pharmacy, Mansoura University, Mansoura 35516, Egypt [2]한국과학기술연구원(KIST) 바이오소재연구센터

A novel series of 2,5-disubstituted-1,3,4-oxadiazole containing amide linker were designed and synthesized. Their in vitro antiproliferative activities were examined over a panel of 60 cancer cell lines of 9 different cancer types at the National Cancer Institute (NCI, Bethesda, Maryland, USA). The compounds tested showed promising anticancer activity. At a single dose concentration of 10 ?M, many target compounds exhibited broad-spectrum anticancer activity over different cell lines of different cancer types. In addition, one derivative was selective against SR leukemia cell line.

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

실리카 나노 입자의 용해도 향상을 위한 실리카-계면활성제 합성

이상윤 김상욱* 김태운 김건균

동국대학교 신소재화학과

실리카 계열의 나노 입자는 페이트, 플라스틱, 전자재료, 흡착제, 건조제 등 다양한 기능성 무기소재 및 의약학 분야에서 약물 전달체 등으로 널리 연구되고 있다. 본 연구실에서는 실리카 나노 입자를 다양한 크기로 합성한 후 엽산 등의 화학물질을 결합 후 방사성동위원소를 도입해 종양의 진단 또는 치료에 이용될 수 있는 방사성의약품을 개발하고 있다. 실리카 계역의 나노 입자는 안정성 및 화학반응의 용이성 등 다양한 특성을 가졌음에도 불구하고 물에 대한 용해도가 낮은 단점을 가지고 있어 합성된 실리카 나노 입자의 용해도를 높여주기 위해 계면활성제를 도입하고자 본 연구를 수행 하였다. TEOS 를 출발물질로 stoeber 법에 의해 50 nm 크기의 실리카 나노 입자를 합성한 후에, 표면을 아민기로 개질하였다. 개질된 나노입자와 개질되지 않은 나노 입자를 대상으로 각각 4, 10, 16%의 TWEEN 60 와 반응 시킨 후 각각의 용해도를 측정하였으며, 분광학적 분석 장비와 주사전자현미경 (SEM) 등을 이용해 합성 여부를 확인 하였고, Zeta sizer 를 이용해 수화 크기를 측정하였다.

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

양전자방출단층촬영용 Sc-44 표지 HBED-CC 방사성의약품 개발을 위한 Sc-45 HBED-CC 합성 및 평가

최평석 김상욱*

동국대학교 신소재화학과

양전자 방출 핵종인 Sc-44 는 Ga-68 과 같이 방사성동위원소 발생장치 Generator 를 통해 쉽게 생산이 가능하고 Ga-68($t_{1/2}$:68 분) 보다 반감기가 약 3 배 길어 Ga-68 의 단점을 보완 할 수 있다. 양기능성 킬레이트제인 HBED-CC (N,N′-bis[2-hydroxy-5-(carboxyethyl) benzyl] ethylenediamine-N,N′-diacetic acid)는 Ga-68 과 표지 시 기존에 사용 되었던 DOTA (1,4,7,10-Tetraazacyclododecane-1,4,7,10-tetraacetic acid), NOTA (1,4,7-triazacyclononane-1,4,7-triacetic acid) 킬레이트 보다 구조적 안정성과 반응성이 높고 암세포 섭취율과 혈류 내 제거 속도가 더 뛰어난 것으로 보고된 바 있다. 따라서 Sc-44 를 HBED-CC 에 표지 하여 PET 진단용 방사성의약품으로 사용한다면 Ga-68 에 표지된 물질 보다 더 효율적일 것으로 사료된다. 이에 기준물질로 안정동위원소인 Sc-45 로 ^{45}Sc-HBED-CC 착화합물을 온화한 조건에서 합성하였고 semi-prep HPLC 로 화합물을 분리하였다. 이후에 RP-HPLC 와 ^{1}H-NMR, LC/MS 를 이용하여 표지 여부 확인 및 표지수율을 측정 하였다. 그 다음 ^{45}Sc-HBED-CC 의 구조적 안정성을 확인하기 위해 2 시간 동안 37℃의 PBS(pH7)와 사람혈청 안에서 안정성을 측정하였고 차례로 ^{45}Sc-HBED-CC 의 신체 내 배설경로를 예측하기 위해 지용성 평가를 실시함으로서 Sc-44 표지 HBED-CC 착화합물의 방사성의약품으로서의 활용 가능성을 연구하였다.

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

Construction of Drug-like 1,3,4-Thiadiazole Libraries via Desulfurative Cyclization of Thiosemicarbazide Intermediate on Solid-phase

최지혜 양승주 공영대*

동국대학교 화학과

Solid-phase synthesis has become an extremely powerful techgnique for the generation of drug-like, small, organic molecule libraries in medicinal chemistry programs. Among organic small molecules, five-membered ring heterocyclic compounds have attracted especially in combinatorial chemistry since they have a wide range of interesting biological activities. In a preceding study, 1,3,4-oxadiazole analogues shown potent biological activity in Wnt signaling which has been regulate cell proliferation, differentiation and morphogenesis. In this respect, we have a interest in synthesis both 1,3,4-oxadiazole and 1,3,4-thiadiazole as a bioisostere. However, we couldn't obtain 1,3,4-thiadiazole analogues selectively in our previous study. In this reason, we tried to develop another synthetic method. Herein, we report our new synthetic strategy to synthesize 1,3,4-thiadiazole analogues on the solid-phase. And substitution reactions with some electrophiles such as alkyl halide and acid chloride generate N-alkylamino and N- acylamino-1,3,4-thiadiazole.

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발표분야: 의약화학
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Synthesis of 3-Substituted-5-Amino-1,2,4-Thiadiazoles via Copper-Catalyzed N-S Bond Formation

김하영 곽세훈 공영대*

동국대학교 화학과

Among organic small molecules, heterocyclic compounds have received particular attention, because they are found in a myriad of bioactive compounds. Thus as a part of an ongoing drug discovery process, we have been studying the synthesis of 1,2,4-thiadiazole derivatives that exhibit a wide range of important biological activities by using both solution and solid phase synthesis. Common approaches to the 1,2,4-thiadiazole from the imidoyl thiourea skeleton are achieved by using coupling reagents or oxidants such as p-toluenesulfonyl chloride, diethyl azodicarboxylate (DEAD), diisopropyl azodicarboxylate (DIAD), bromine, N-chlorosuccinimide, hydrogen peroxide and HCl for the formation of N-S bond, which would produce undesired products or wastes inducing purification to be tricky. Instead of these classical methods, we here wish to report the synthesis 1,2,4-thiadizoles by oxidative copper-catalyzed N-S bond formation.

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발표분야: 의약화학
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Construction of a Novel *N*,*N*',*N*"-Trisubstituted-guanidine Derivatives as anti-Inflammatory Agents

이지형 최용문[1] 공영대[*]

동국대학교 화학과 [1](재)경기과학기술진흥원 연구개발팀

Inflammation is a kind of immune response such as pathogens, damaged cells, or irritants and a protective attempt by the organism to remove the injurious stimuli. Chronic inflammation can also lead to a host of diseases, such as hay fever, periodontitis, atherosclerosis, rheumatoid arthritis, and even cancer. Asthma is a common chronic inflammatory disease of the airways characterized by variable and recurring symptoms, reversible airflow obstruction, and bronchospasm. And heterocyclic compounds are commonly used scaffolds on which pharmacophores are arranged to provide potent and selective drugs. This is especially true for five-membered heterocyclic compounds, which serve as the core components of many substances that possess a wide range of interesting biological activities. In that regard, we concentrated our effort to construction of a novel small organic drug-like lead compound without side-effect of existing anti-inflammatory drugs. As a result, we synthesized *N*,*N*',*N*"-trisubstituted-guanidine derivatives via heterocyclic thiourea intermediate with various aromatic amines.

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Synthesis of N-alkyl, N-acyl, and N-sulfonyl-2-aminobenzo[d][1,3]thiazine Derivatives on BAL Resin

김은미 이지형 공영대*

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The small and simple benzo[d]thiazine nucleus possesses numerous biological properties like - antitumor, cardiovascular, neurodegenerative pathologies, antiproliferative activity. These activities are also possessed by its substituted derivatives as well. Also solid-phase synthesis of combinatorial libraries has emerged as a powerful tool for efficient drug discovery process. A novel solid-phase methodology has been developed for the synthesis of N-alkyl, N-acyl, and N-sulfonyl-2-aminobenzo[d]thiazine derivatives. These core skeleton 2-aminobenzo[d]thiazine resins undergo functionalization reaction with various electrophiles, such as alkyl halides, acid chlorides, and sulfonyl chlorides to generate N-alkyl, N-acyl, and N-sulfonyl-2-aminobenzo[d]thiazine resins, respectively. Finally, 2-aminobenzo[d]thiazine derivatives are then generated by cleavage of the respective resins under trifluoroacetic acid (TFA) in dichloromethane (DCM).

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Synthesis of 2,3-Diaminobenzo[b]thiophenes via Intramolecular C-S Bond Formation of Ugi Adducts

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Multi-component reactions (MCRs) have gained much attention in drug discovery research as the reactions facilitate preparation of variable and complex compounds with ease from simple starting materials. In addition, the products from MCRs can be also further transformed into valuable chemicals. This strategy was also conducted using Ugi adducts to generate a diverse heterocycles, attractive targets for medicinal chemistry research. In this regard, we prepared prefunctionalized Ugi adducts from reactions with aldehydes, isonitriles, amines, and sulfinic acids. The adducts were cyclized via intramolecular C-S bond formation to give 2,3-substituted diaminobenzo[b]thiophenes, which could not be easily obtained by other routes.

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Construction of a Drug-like 2,5-Piperazinedione Derivatives by Microwave-assisted Synthesis

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Heterocyclic compounds are commonly used as scaffolds on which pharmacophores are arranged to provide potent and selective drugs. This is especially true for six-membered ring heterocyclic compounds, which are core components of various substances that possess a wide range of interesting biological activities. The piperazinedione is of significant interest in biology and drug discovery. Its unique heterocyclic system found in several natural products constitutes a rich source of new biologically active compounds. For example, the piperazinedione derivatives display antitumor, antiviral, and antifungal activity. Many modern programs of medicinal chemistry exploit combinatorial methods (i.e., the simultaneous or parallel synthesis of libraries, and their subsequent screening) to speed up drug discovery. Along these lines, we have devoted our efforts to develop a solution-phase strategy for the preparation of a small molecule library of the piperazinedione. Here, we report a useful method for the synthesis of 1-(1,3,4-oxadiazol-2-yl)piperazine-2,5-dione derivatives.

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Synthesis of Ga-68 labeled new radiopharmaceuticals for tumor diagnosis

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동국대학교 화학과

Recently, the design of surface-modified nanoparticles have been interested greatly in nanobiotechnology (NBT) due to the major applications, such as contrast media.Among the various nanoparticles, iron oxide was used to have applications in tagging for biosensing, probe of drug delivery and contrast media for magnetic resonance imaging (MRI).This research was focus on developing of nano-bio targeting composites using Fe_3O_4 nanoparticles and Ga-68 radioisotope, which could be useful for therapy in hyperthermia and diagnosis in the fields of PET and MRI applications. The surface of Fe_3O_4 nanoparticles that are used MRI imaging and hyperthermia can be reformed by citric acid to increase hydrophilic property. Nano-bio targeting composites can be obtained by combining Fe_3O_4 nanoparticles and NOTA as bifunctional chelating agent with Ga-68 radioisotope,This bi-functional imaging media will allow the earlier detection of tumor with a high degree of accuracy.

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Preparation of heteroaryl piperazine libraries as plausible kinase inhibitors

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Heteroaryl rings containing N are the most privileged scaffolds for kinase inhibitors. A series of heteroaryl compounds with piperazine linker to improve druggability including solubility were prepared as plausible kinase inhibitors. Quinoxalin-2-yl-, quinolin-3-yl-, isoquinolin-3-yl-, quinazolin-4-yl-, benzo[d]imidazol-2-yl-, benzo[d]thiazol-2-yl-, benzo[d]oxazol-2-yl-,pyrimidin-2-yl-, and pyridine-2-yl-piperazines were synthesized using a variety of starting materials and further diversified. The compounds with linkers including diazepine, substituted piperazine, piperidine were additionally prepared. The synthesized compounds are currently using as focused kinase libraries.

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파낙스속 식물의 신규가공법 개발과 유효성분의 극대화 연구

최필주 김영석 주해윤 전상일[1] 함정엽[2,*]

강릉원주대학교 화학신소재학과 [1]강릉원주대학교 화학과 [2]한국과학기술연구원(KIST) 천연의약센터

인삼은 식물분류학상 오갈피나무과 파낙스속에 속하는 다년생 숙근초로, 오래 전부터 한약처방에서 중요한 약재로 사용되어 왔다. 최근에는 인삼을 장기간 저장하고 유효성분을 높이기 위한 목적으로 수증기 또는 기타 방법으로 증숙하여 인삼의 전분을 호화시켜 건조하여 홍삼을 제조하여 사용해 왔다. 인삼과 홍삼의 약리작용은 사포닌 배당체인 Ginsenoside 에 의해 나타나는 데 약 40 여종이 보고되었다. 그 중 홍삼에만 포함된 Ginsenoside 인 Rg3, Rk1, Rg5 는 기존 인삼과 비교하여 항암활성이 월등하고 혈관이완작용, 혈소판 응집억제 효과 등의 새로운 약리활성이 많이 보고되었다. 그로 인해 유효 Ginsenoside 의 함량을 높이기 위한 방법에 대해 연구가 이루어 지고 있지만 새로운 방법을 제시하지 못하고 있다.이에 본 연구에서는 인삼추출물을 새로운 가공 방법을 통해 인삼의 유효성분인 Ginsenoside Rg3, Rk1, Rg5 의 함량을 극대화 하는 데 있다.

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Synthesis of F-18 labeled benzopyran derivative

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동국대학교 화학과

The over stimulation of the glutamate receptor system (N-methyl-D-aspartate receptor) causes neurodegeneration due to a process called excitotoxicity such as Alzheimer's disease (AD). AD is the most common cause of dementia in the geriatric population. Benzopyran derivatives have a therapeutic effect on neurodegenerative diseases. In this study, we synthesized the F-18 labeled benzopyran derivative for neurodegeneration. The target compound was synthesized starting from 2-hydroxy-5-nitroacetophenone in six steps as a novel potential Positron emission tomography (PET) radiotracer for the diagnosis of neurodegenerative disorders. Further pharmacological investigation of F-18 labeled benzopyran derivative is in progress.

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Natural Products Based Drug Development: The Concept of Naturomimetic Approach Method

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Recently, natural products obtained from the nature exhibit a lot of biological activities and it sometimes become to the lead compound for drugs. For example, natural products and its derivatives such as Taxol, Vincristine, Morphine and Codeine are already used as anticancer drugs and anodynia, and so on. Especially, these natural products are suitable in terms of safety for human, therefore, drug development from natural products has received much attentions in the world. Focusing on new drug development, we have been continuing to synthesize pharmacophores of natural products including biological activities and further modifying them to functionalized derivatives. Also, to further enhance effective methods to find natural product derivatives, our research has applied to the concept of Naturomimetic Approach developed by our group. Biologically active pharmacophore of natural product is synthesized and efficient research to find further moiety is conducted through C-C/C-N coupling, Click reactions utilizing general methods. In the poster presentation, we will introduce the concept of Naturomimetic Approach method.

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Natural Products Based Drug Development: Recent Results in Naturomimetic Approach Method

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Recently, natural products obtained from the nature exhibit a lot of biological activities and it sometimes become to the lead compound for drugs. For example, natural products and its derivatives such as Taxol, Vincristine, Morphine and Codeine are already used as anticancer drugs and anodynia, and so on. Especially, these natural products are suitable in terms of safety for human, therefore, drug development from natural products has received much attentions in the world. Focusing on new drug development, we have been continuing to synthesize pharmacophores of natural products including biological activities and further modifying them to functionalized derivatives. Also, to further enhance effective methods to find natural product derivatives, our research has applied to the concept of Naturomimetic Approach developed by our group. Biologically active pharmacophore of natural product is synthesized and efficient research to find further moiety is conducted through C-C/C-N coupling, Click reactions utilizing general methods. In the poster presentation, we will introduce our recent research results in Naturomimetic Approach Method derived from Amorphstilbol, Justicidins, Guggulsterone and so on.

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Synthesis of new triazolo[4,5-*d*]pyrimidine derivatives as potential antitumor agents

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New triazolo[4,5-*d*]pyrimidine derivatives were synthesized. Their *in vitro* antitumor activity was evaluated using at National Cancer Institute, USA. Most compounds displayed growth inhibitory activities on leukemia, melanoma, lung, colon, CNS, ovarian, renal, prostate, and breast cancer cell lines. Leukemia (K-562 and SR), Non-Small Cell Lung Cancer HOP-92, Melanoma MDA-MB-435 and Renal Cancer A498 were found to be the most sensitive cell lines. Compound 21 proved lethal to Non-Small Cell Lung Cancer HOP-92 while it showed remarkable growth inhibitory activities against Leukemia K-562 and Melanoma MDA-MB-435 with GP values of 27.12 and 23.78% respectively. Compound 23 inhibited growth of Non-Small Cell Lung Cancer HOP-92 with GP value of 12.34%.

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Synthesis and SAR of urotensin-II receptor (UT) antagonists

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The urotensin-II ligand (U-II) is a cysteine-linked cyclic undecapeptide and is known as one of the most potent vasoconstrictor. The U-II is widely expressed in the peripheral vasculature, heart and kidney with high level. The interaction of U-II with a specific G protein-coupled receptor, urotensin-II receptor (UT), exerts its effect to play an important role in the regulation of cardiorenal function. As the based on the previous results of UT function on biological and pharmaceutical study, UT would be a promising target for treatment of cardiovascular diseases, especially heart failure. As part of drug discovery project in the development of novel and potent UT antagonists, we recently have identified a series of aminopiperidine derivatives as hit compounds. In an continuing effort to optimize for these compounds, we investigated the effects of various substituents on heteroaryl containing the aminopiperidine group to the UT binding activity. The details of synthesis and structure-activity relationships (SAR) results will be discussed.

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Regioselective Synthesis of 1,3,4-Oxadiazole and 1,3,4-Thiadiazole Analogues via Reagent-based Cyclization of Thiosemicarbazide Intermediate

양승주 서진호 공영대*

동국대학교 화학과

Heterocyclic compounds are commonly used scaffolds on which pharmacophores are arranged to provide potent and selective drugs. This is especially true for five-membered ring heterocyclic compounds, which serve as the core components of many substances that possess a wide range of interesting biological activities. In this family, 1,3,4-oxadiazoles and 1,3,4-thiadiazoles have been used as “privileged” scaffolds to produce substances of interest in numerous therapeutic areas, such as anti-inflammatory, anti-microbial, anti-convulsant, anti-cancer, and anti-hypertensive. In this reason, we established synthetic methodology for the synthesis of 1,3,4-oxadiazole and 1,3,4-thiadiazole analogues. The resulting 2-amino-1,3,4-oxadiazole and 2-amino-1,3,4-thiadiazole core skeleton are functionalized with various electrophiles such as alkyl halide, acid halides, and sulfornyl chloride in high yields.

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Epigenetic Activation and Stabilization of RUNX3 through Posttranslational Modification and Lactam-Based HDAC Inhibitors: Novel Insight of Epigenetic Anticancer Approach

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Runt-related transcription factor 3 (RUNX3), a tumor suppressor, functions as the functional inactivation of RUNX3 is related to tumor development. Histone deacetylase (HDAC) inhibition can restore expression of RUNX3 in transcriptional level and in posttranslational level. However, strong induction of RUNX3 mRNA at the transcription level and altered gene expression profiles can cause nonspecific gene expression. In-house chemical library of 111 lactam-based HDAC inhibitors were screened to identify potent RUNX3 stabilizers through acetylation. RUNX activity and HDAC inhibition were determined by a cell-based RUNX activation and HDAC inhibition assay. Three candidate compounds: 11-8, 11-48, 11-58 were selected as they showed significantly increased acetylation and stability of RUNX3. Among the three, 11-8 was the most suitable anticancer agent with relatively low RUNX3 mRNA expression and moderate HDAC inhibitory activity. This compound also showed significant antitumor effects, which were stronger than SAHA, in an MKN28 xenograft model. Thus, we propose a novel approach, in which HDAC inhibitors serve as antitumor chemotherapeutic agents that selectively target epigenetic regulation and protein stability of RUNX3.

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Identification of Thienopyrimidine-based FLT-3 Inhibitors By Chemical Rearrangement From the Kinase Inhibitor Library

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For years, researches on the relationship between proinflammatory cytokines and related diseases revealed that proinflammtory cytokines, particularly NF-κB, are responsible in inducing excessive inflammatory responses in the body. Inhibition of production of NF-κB has been a popular approach to treat auto-immune diseases such as rheumatoid arthritis. In this paper, identification of thienopyrimidine analogues is focused on small molecules through modification of the known IKKβ inhibitor, SPC-839. There, however, no inhibitory activity against IKKβ was observed with these compounds. These thienopyrimidine-based compounds were then screened for a new target kinase, and as a result, FLT3 was identified as the potential target of these compounds. FLT3 (Fms-like tyrosine kinase 3), a receptor tyrosine kinase, is a member of receptor III tyrosine kinase family and in charge of development of the immune system. Thienopyrimidine-based compounds showed good inhibition tendency against FLT3 even under 1 μM treatment. In conclusion, these compounds have the potential to be the future therapeutic solutions for treatment of AML through the specific inhibitory functioning on FLT-3.

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Development of selective 5HT2c radioligands for PET neuroimaging

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Serotonin (5-hydroxytryptamine, 5-HT) is one of the monoamine neurotransmitters in the human brain to be involved in regulation of various psychological conditions such as appetite, libido, pain, and biorhythm. It is mediated by multiple receptor subtypes that have been classified into seven subfamilies (5-HT1 to 5-HT7). Among them, the 5-HT2 receptor belongs to the large family of GPCR (G protein coupled receptors) and consists of 5-HT2a, 5-HT2b, and 5-HT2c. The 5-HT2c receptor is related to diverse brain diseases including obesity, anxiety, depression and schizophrenia and yet has attracted less attention in psychopharmacology and neuroimaging than the other receptors. In particular, this receptor is associated with the physiological regulation of the mammalian sleep?wake cycle, whereby it is pivotal to the interaction model of non-rapid eye movement (NREM)/REM sleep stage cycling. In order to identify the role of the 5-HT2c receptor in the sleep disorder, development of an in vivo method for measuring its function and density is important and the PET (positron emission tomography) imagining might be one of the potential tools for this purpose. Currently, many selective ligands exist for 5-HT2c, but have not been evaluated as PET radiotracers.In this study, we have synthesized pyrimidine derivatives as selective 5-HT2c PET imaging agents for the study of the sleep disorder. We successfully synthesized an arylstannane precursor for fluorine-labeling, which was subjected to a fluoride-promoted aryl exchange reaction via a diaryliodonium salt to afford the desired target pyrimidine after HPLC separation. The result of radiofluorination and its in vivo function will be discussed in this presentation.

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Hybrid Hsp90 inhibitors and their anti-proliferative effects against gefitinib-resistant non-small cell lung cancer (NSCLC)

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Over the past two decades, several targeted drugs have been discovered to eradicate cancers in specific ways and reduce the harmful nonspecific side effects of conventional chemotherapeutics. However, this notion of single targeted therapy has been challenged by the emergence of drug resistance. The tumor cells outsmart single-targeted drugs to escape from their destiny by mutating targeted proteins, down-regulating death signals, or up-regulating survival pathways. Heat shock protein 90 (Hsp90) is an ATP-dependent chaperone that is responsible for the folding, activation, and stabilization of numerous client proteins. Hsp90 has become an attractive therapeutic target in cancer research. Many Hsp90 client proteins play significant roles in six essential hallmarks of cancer cell, including Akt, Raf-1, mutant p53, Cdk4, VGEF, MET and HIF-1α. The therapeutic potential of targeting Hsp90 may be best appreciated by simultaneously attacking the six hallmarks of cancer cells. Accordingly, the inhibition of Hsp90 function promotes ubiquitin-dependent proteasomal degradation of its client proteins, which can eventually lead to cell death. Besides, Hsp90 is expressed at 2-10 fold higher levels in tumor cells compared to their normal cells.As part of our ongoing efforts to discover small molecules targeting N-terminal ATP-binding pocket of Hsp90, we had performed a structure-based drug design (SBDD) of small molecule inhibitors against Hsp90. Designed inhibitors were synthesized and their anti-cancerous activities were evaluated. Here, we report our effort to develop therapeutic agents against Hsp90 in cancer.

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Synthesis of flavokawain B and its analogues and their inhibitory effect on Hsp90 machinery

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Non-small cell lung cancer (NSCLC) is the most common type of lung cancer and that is responsible for 85% of lung cancer patients. Despite several EGFR inhibitors have been developed in the treatment of NSCLC, the clinical efficacy of EGFR inhibitors in NSCLC is limited by the development of drug-resistance through the mutation of EGFR and the overexpression of Met. Hsp90 is an ubiquitous molecular chaperone protein, which accounts for 1-2% of the cytosolic protein under non-stressed conditions. Hsp90 plays an important role in regulating maturation and stabilization of many oncogenic proteins in six essential hallmarks of cancer, including EGFR, Her2, Met, Akt, Raf, HIF-1 and MMP2. In this regard, Hsp90 represents great promise as a therapeutic target of cancer due to its potential to simultaneously disable multiple signaling pathways. Considering both EGFR and Met are client proteins of Hsp90, to block Hsp90 protein folding machinery may be best suited to overcome the resistance from EGFR mutation and Met amplification.Kava (Piper methylsticum) is a native plant traditionally used as a medicine and social drink in the South Pacific islands, including Fiji, Vanuatu and Western Samoa. Flavokawain B, one of chalcone component isolated from kava extract, has been reported to exhibit strong anti-proliferative effects against several cancer cell lines. In this study, we discovered that a natural product, flavokawain B and its analogues disrupted Hsp90 chaperoning function and impaired the growth of gefitinib-resistant non-small cell lung cancer (H1975). The result suggested that flavokawain B and its analogues could serve as a potential lead compound to overcome the drug resistance in cancer chemotherapy.

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Activity and Selectivity Studies of 4-Phenylpiperazine Derivatives on D2-like Dopamine Receptors using 3D-QSAR and Docking Methods

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The D2-like dopamine receptors are associated with neuropathological disorder such as schizophrenia, drug addiction and Parkinson’s disease. It is difficult to design the subtype-specific compounds to reduce side-effects because of high homology among subtype receptors. In this study, we identify activity and selectivity factors of D2-like receptor with 4-phenylpiperazine derivatives using computational method such as 3D-quantitative structure activity relationship (3D-QSAR), molecular docking and homology modeling. Three activities of D2, D3, D4 subtype and two selectivity of D4 versus D2 or D3 subtype 3D-QSAR models show a good correlation (r2) of 0.96, 0.91, 0.94 for activity and 0.87, 0.95 for selectivity, and a reliable prediction value (Q2) of 0.51, 0.80, 0.56 for activity and 0.43, 0.79 for selectivity, respectively. We defined properties and position of substituent to increase an activity or a selectivity by analysis of contour map based on electrostatic potential field and van der Waals field. Moreover, key residues, Ser2.64 and Phe2.61 of D4, Tyr1.39 of D3 and Leu1.39 of D2 subtype, are elucidated by a different binding mode of highly active compounds on subtypes from docking studies. Additionally, we found selectivity for D4 subtype that are also caused by susceptible region where restricted hydrophobic space from hydrogen bond between amine of pyrazole moiety and hydroxyl group of Ser2.64. In conclusion, we identify that a favorable property of substituent to increase activity for subtype and D4-selectiviy from 3D-QSAR models as well as both key residues and conformational selectivity to affect different binding modes from docking studies. These results will support to design selective drugs on D2-like dopamine receptors.

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Development of cholinesterase inhibitors using 1-benzyl piperidin-4-yl and 1-benzyl piperazin-4-yl (R)-lipoic amide molecules

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한밭대학교 생명공학과 [1]한밭대학교 생유기화학실험실 [2]한밭대학교 응용화학과 [3]한밭대학교 응용화학 [4]한밭대학교 응용화학생명공학부

A series of hybrid molecules between (R)-lipoic acid (ALA) and 4-amino-1-benzyl piperidines and 1-benzyl piperazines were synthesized and their in vitro cholinesterase (acetylcholinesterase (AChE) and butyrylcholinesterase (BuChE)) inhibitory activities were evaluated. Even though the parent compounds did not usually exhibit any inhibitory activity against cholinesterase (ChE), hybrid molecules demonstrated BuChE inhibitory activity. Some hybrid compounds also displayed AChE inhibitory activity. Specifically, N-(1-benzylpiperidin-4-yl)-5-(1,2-dithiolan-3-yl)pentanamide (AChE (IC50 = 1.75±0.30 μM) and BuChE (IC50 = 5.61±1.25 μM)) and 5-(1,2-dithiolan-3-yl)-1-(4-(3-methylbenzyl)piperazin-1-yl)pentan-1-one (AChE (IC50 = 30.3 ± 0.6 μM) and BuChE (IC50 = 2.3 ± 0.7 μM)) were shown to be an effective inhibitor against both and comparable to galantamine (IC50 = 1.7±0.9 μM against AChE and IC50 = 9.4±2.5 μM against BuChE).

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First Identification of Novel Chemotypes for TREK1 Antagonists by an Integrated Structure- and Ligand-based Rational Approach

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Although TREK1 (Twik-RElated Potassium (K+) channel 1) is a well-characterized target for several neuronal disorders, the species-specific inhibitors are scarce. This study has been carried out with the objective of finding novel chemotypes by an integrated structure- and ligand-based rational approach. We firstly built the homology model of TREK1 and testified as reliable for employing in further research. In order to select the most accurate software for our lead discovery process, the 3D model was subjected to a comprehensive docking campaign with quaternary ammonium compounds (QAs) using CDOCKER, SURFLEX, GLIDE and GOLD programs, the best one which makes a good consensus of theoretical results with TREK1 inhibition data, was chosen. We try to gain further insights into the key binding interactions between the protein and ligands by docking of 26 known antagonists (with a specific inhibitory activity for TREK1) with the hypothetical structure. Guided by this information, a common feature-based pharmacophore model (Hypo1) was generated for six active (0.1 ?M ≤IC50≤1 ?M) compounds from the antagonists discussed here. Validated Hypo1 and the most potent compound (IC50 0.06 ?M) in the data set were employed as pharmacophore- and 2D similarity-based queries respectively, for the virtual screening of commercial libraries. The retrieved hits were prioritized by applying drug-like property filters and docking, top scored 33 compounds were selected and purchased. Subsequent in vitro study has identified 11 propitious lead compounds with 9 distinct chemotypes, in which, compound 1 showed significant TREK1 inhibition of 54% at 10 ?M and an IC50 of 13.30±4.03 ?M and others had an inhibition rate of 25-39%.

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Discovery and Biological Evaluation of Novel 18 kDa Mitochondrial Translocator Protein (TSPO) Ligands for the Treatment of Alzheimer's Disease

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과학기술연합대학원대학교(UST) 의약 및 약품화학 [1]한국과학기술연구원(KIST) 생체과학연구본부

The role of mitochondrial β-Amyloid peptide (Aβ) has been highlighted in Alzheimer's disease (AD) pathogenesis by its interaction with cyclophilin D (CypD). CypD, adenin nucleotide translocator (ANT), voltage-dependent anion channel (VDAC), and 18 kDa translocator protein (TSPO) compose the mitochondrial permeability transition pore (mPTP). Aβ enhances both mPTP opening and influx of cytosolic solutes into the mitochondrial matrix. Consequently, Aβ can cause mitochondrial swelling and apoptotic cell death. The 18 kDa TSPO ligand inhibiting mPTP can be an effective therapeutic strategy in AD. Based on the pharmacophore-based virtual screening, we identified novel TSPO ligand scaffolds and their biological evaluations were performed. They showed effective biological properties in five in vitro cell-based assays; JC-1, ATP production, MTT, Calcein AM, and ROS inhibition assays. The in vivo assay results of the Y-maze spontaneous alternation test in a mouse model of AD also showed that the novel TSPO ligands improved memory and cognitive functions. Through the optimization process, more than 100 derivatives were synthesized and their biological properties were measured by five in vitro cell-based assays. And then, selected compounds were injected into Aβ-induced acute AD mouse model for the behavioral test. Especially, two compounds out of the derivatives showed therapeutic effects on both in vitro and in vivo assays. In the poster presentation, we will suggest the 18 kDa TSPO as a therapeutic target for AD as well as the biological results of TSPO ligands that we have researched so far.

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Efficient Synthesis of Sulfonamide Substituted Thiophene

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고려대학교 화학과 [1]한국화학연구원 신물질연구단 난치성질환치료제연구센터

Thiophene is known to play a crucial role in the metabolic activation of various thiophene-containing drugs. Sulfonamide substituted thiophene have been attracting much interest key moieties for the synthesis of biologically active compounds. We studied mild condition used oxime-protection for produce the thiophene derivatives in the industrial way.

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Synthesis and Antitubercular Activity of Bicyclic Nitroimidazole Carbamate Derivate

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성균관대학교 화학과 [1]한국화학연구원 신약연구단 [2]한국화학연구원 신물질연구단 난치성질환치료제연구센터

Recently the re-emergence of tuberculosis (TB) in the world wide, accompanied by the rise of multidrug-resistant (MDR) strains, emphasizes the need for the discovery of new therapeutic drugs with greater efficacy, safety and novel mechanism of action against this disease. The PA-824 ((6S)-2-nitro-6-{[4-(trifluoromethoxy)benzyl]oxy}-6,7-dihydro-5H-imidazo[2,1-b][1,3]oxazine) containing nitroimiazole has entered phase II clinical trials as novel TB therapeutics. The mechanism of action of PA-824 involved as mycolic acid synthesis inhibitors and intracellular nitric oxide (NO) release for respiratory poisoning under aerobic and anaerobic conditions. We synthesized bicyclic nitroimidazole carbamete derivate had better inhibitory effect for antituberculosis than conventinal monocyclic nitro imidazole compound, particularly excellent inhibitory effect on inactive tuberculosis.

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mGluR1 antagonists for the treatment of neuropathic pain

selvarajmuthusamy **배애님[1,*] 남길수[2,*] 최경일[3,*]**

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Abstract:Metabotropic glutamate receptor 1 (mGluR1) plays an important roles in the neurotransmission and pathogenesis of several neurological disorders, neuropathic pain including chronic pain. Antagonists of mGluR1 have been suggested to be useful for the treatment of pain. We found a hit compound from a screening of a library of compounds for mGluR1 (89.22% inhibition at 10 μM). The compound has tetrahydroquinazoline structure and contained indanamino and hydroxyethylthio substituents. To find more effective inhibitors, we varied the substituents of KKJD0001, and found KKJD0005 as the best of the derivatives we synthesized (81.11% inhibition at 10 μM). The compound KKJD0005, however, showed moderate activity in vivo.

mGluR1 antagonists for the treatment of neuropathic pain

Selvaraj Muthusamy,[a,b] Ae Nim Pae,[a,b] Ghilsoo Nam,[a,b] and Kyung Il Choi[a,b]

Abstract:

Metabotropic glutamate receptor 1 (mGluR1) plays an important roles in the neurotransmission and pathogenesis of several neurological disorders, neuropathic pain including chronic pain. Antagonists of mGluR1 have been suggested to be useful for the treatment of pain.

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Strain-Promoted Click Chemistry for ^{18}F-labeling of Tetrameric RGD Peptide and microPET Imaging of Tumor Integrin $\alpha_v\beta_3$ Expression

kalme sachin 정현진 김동욱*

인하대학교 화학과

In this study a new ^{18}F labeled tetrameric RGD Peptides have been developed for PET of integrin expression, using the strain-promoted azide and alkynes cycloaddition reaction and subsequent chemo-orthogonal purification reaction proceeded fast and selectively under physiologically friendly reaction condition which gives a high specific activity with high radiochemical yield. This ^{18}F-labeled tumor targetable bioactive peptide cRGD$_4$-PEG$_4$-ADIBOT- ^{18}F was subjected to microPET studies in U87MG xenograft models. Showed rapid and higher tracer uptake in U87MG tumors and relatively good metabolic stability, as well as favorable in vivo pharmacokinetics. We expect that the reaction condition presented here will widen the application of the click reaction for the preparation of ^{18}F-labeled peptides to various types of biomolecules for future microPET Imaging of Tumor Integrin $\alpha_v\beta_3$ expression.

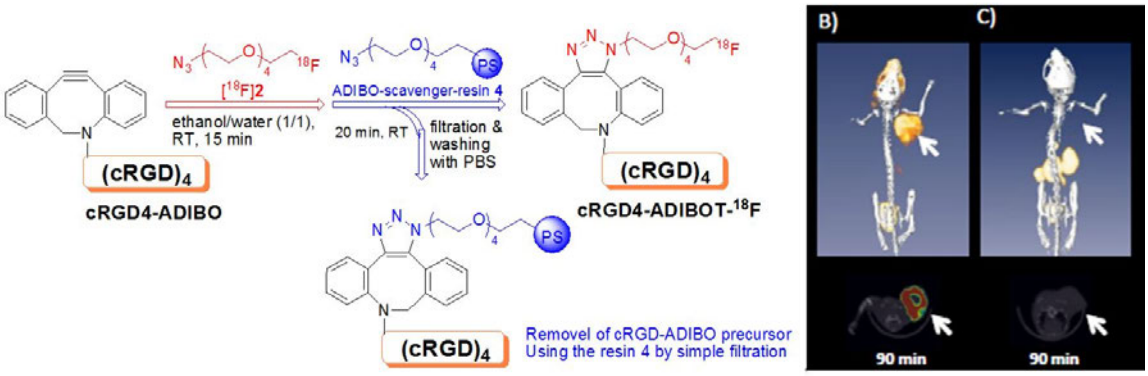

Figure 1. A) Synthesis of F-18 labelled (cRGD)n based on chemo-orthogonal SPAAC reaction protocol; microPET-CT images of U87MG tumor bearing mice at 90 min post-injection of 1.8 MBq of cRGD4-PEG4-ADIBOT-^{18}F without (B) and with (C) (denoted as "Blocking") a co-injection of nonradioactive cRGD4-PEG4-ADIBOT-F. Tumors are indicated by white arrows.

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Anti-oxidative and anti-cholinesterase activities of organic extracts of Propolis produced from Korea and China

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In our continuing search for anti-oxidative and anti-cholinesterse compounds from natural resources, we examined Propolis produced from Korea and China and compared their activities each other. Thus here we report the progress on the purification and biological activities of the partially purified fractions. From the 100 % methanol extracts of Korean and Chinese Propolis, solvent partition fractions were prepared by using n-hexane, chloroform, butanol and water, and among them chloroform fraction showed anti-oxidative and BuChE inhibitory activities. The chloroform fraction of Korean Propolis showed about 84.3% DPPH radical scavenging activity and 80.0% BuChE inhibitory activity at 0.1 mg/mL, and the chloroform fraction of Chinese Propolis also showed similar activities (83.5% DPPH radical scavenging activity and 66.6% BuChE inhibitory activity at 0.1 mg/mL). Using various chromatographic methods and by the bioassay-guided fractionation, the chloroform fraction of Korean Propolis was separated into four fractions, and each fraction showed anti-oxidative activity as 77.4, 84.2, 83.6, 82.0% at 0.1mg/mL, and anti-BuChE activity as 73.9, 77.5, 79.3, 70.2% at 0.1mg/mL, respectively. Similarly, the chloroform fraction of Chinese Propolis was separated into four fractions, and each fraction showed anti-oxidative activity as 70.9, 82.5, 82.9, 77.9% at 0.1mg/mL, and showed anti-BuChE activity as 77.7, 89.9, 91.9, 80.4% at 0.1mg/mL, respectively. So far, both Korean and Chinese Propolis did not show any significant difference both in biological activities and TLC pattern. Purification, structure determination, their biological activities of the purified compounds are to be reported.

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Iodoemodin을 이용한 유방암 세포주에 대한 형광면역학적 평가

박정훈 이준영[1] 허민구 양승대*

한국원자력연구원 방사선기기연구부 [1]동국대학교 신소재화학과, 한국원자력연구원 방사선기기연구부

지난 연구를 통해 방사성동위원소 I-123 이 표지된 emodin (3-methyl-1,6,8-trihydroxyanthraquinone)이 유방암에 과발현되어 있는 HER-2 수용체를 특정적으로 결합하는 특징을 확인하였다. 본 연구에서는 emodin 에 안정동위원소 요오드를 도입하여 형광면역방법을 이용하여 유방암 세포주인 SK-BR-3 에 대한 세포섭취도를 측정하였다. 2-Iodoemodin 은 NaI 용액과 32% peracetic acid 를 이용하여 실온에서 10 분간 교반을 시켜 수행하였으며 ammonium acetate 와 methanol 을 이동상으로 역상-고성능액체크로마토그래피(RP-HPLC)법을 이용하여 Rt=25 분에서 용출되는 iodoemodin 을 분리하였다. 1H-NMR 분광기, 고분해능 고속원자충격 질량분석기 (HR-FAB-MS)를 통해 분자구조 및 분자량을 확인하였다. 유방암 세포인 SK-BR-3 를 1 ×105 개 1 mL 씩 24 well plate 에 넣어 5% CO2, 37℃에서 24 시간동안 성장시켜 well 에 2-iodoemodin 가 기준물질은 emodin 을 농도별로 적가하고 시간별 (15 분, 30 분, 60 분, 120 분)로 phosphate buffered saline (PBS)으로 두 번씩 세척 후 형광측정기를 통해 세포섭취도를 측정하였다. 시간이 증가함에 따라 SK-BR-3 에 대한 세포섭취도가 emodin 에 비해 2-iodoemodin 이 높았으며 형광현미경으로 2-iodoemodin 이 l SK-BR-3 에 섭취되었음을 확인하였다.

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Construction of Multifunctionalized Thiazolo[4,5-e][1,4]diazepine-5,8-dione Library under Solid-Phase Protocol

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경북대학교 약학과 [1]경북대학교 약학대학

Immense pharmacological importance of benzodiazepines, which is the known privileged scaffold, led to a great deal of work on various facets of heteroannelated diazepines. Thus, five-memberd heterocycles fused-diazepines, such as thiophenes, imidazoles, pyrroles, isoxazoles, and pyrazoles, were synthesized and investigated for their pharmacological activity. We have previously reported a traceless solid-phase synthesis of thiazoles and their fused-thiazoles Library. Our current interest in fused-thiazoles prompted us to plan the synthesis of thiazolo[4,5-e][1,4]diazepine-5,8-dione derivatives. The combinatorial synthetic strategy involves the formation of polymer-supported thiazole by the cyclization with cyanocarbonimidodithioate and ethyl 2-(2-halooacetamido)acetate. The thiazolo[4,5-e][1,4]diazepine-5,8-dione moieties are introduced by acid-catalyzed intramolecular cyclization. Finally, traceless cleavage of sulfone linker is achieved with various amine and thiol nucleophiles to give thiazolo[4,5-e][1,4]diazepine-5,8-dione derivatives in good overall yield from the Merrifield resin.

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Parallel Synthesis of Functionalized Thiazole Derivatives on Solid-Phase

김대훈 이두현 이수연 이승연 김태금 이원화 곽소영[1] 이태호[*]

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The combinatorial synthesis of small organic molecules in either the solution-phase or on solid support has had a significant impact in the area of drug discovery. Among small molecule families, heterocyclic compounds have received particular attention in this regard, since they are often important structural components of bioactive molecules. Thiazole Derivatives exhibit a wide range of important biological properties and, as a result, they serve as attractive targets for combinatorial library construction via solid-phase synthesis. The combinatorial synthetic strategy involves the formation of polymer-supported thiazole by the cyclization with cyanocarbonimidodithioate and alpha-haloamides. After the additional diverse moieties are introduced, traceless cleavage of sulfone linker is achieved with various amine nucleophiles to give 2,4-disubstituted-5-aminocarbonyl-1,3-thiazole derivatives in good overall yield from the Merrifield resin.

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Design and Synthesis of Novel (1S)-(-)-verbenone derivatives as potent anti-ischemic agents

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Strokes can be classified into two major categories: ischemic and hemorrhagic. Ischemic strokes are those that are caused by a sudden interruption in cerebral blood supply due to an embolus or a thrombus, while hemorrhagic strokes are the ones which result from rupture of a blood vessel or an abnormal vascular structure. About 87% of strokes are caused by ischemia. Rapid recovery of cerebral blood flow is essential to limit neuronal injury and resultant loss of brain function. Recent research indicate that injury in ischemic regions may advace even after reperfusion. Therefore, the development of agent that treat effectively against this progressive ischemic injury is ardently pursued. A series of novel (1S)-(-)-verbenone derivatives was synthesized referenced from a 4-styryl scaffold and were tested for measuring their anti-oxidant, anti-excitotoxic, and anti-ischemic activites. These derivatives considerably decreased oxygen-glucose deprication-induced neuronal injury and N-methyl-D-aspartic acid-evoked excitotoxicity in cortical neurons. Furthermore, one of these derivatives was confirmed as a potent anti-ischemic agent in in vivo ischemic model, potentially due to the supression of N-methyl-D-aspartic acid-evoked excitotoxicity and oxidative/nitrosative stress. More detailed chemical and pharmacological results will be presented.

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Synthesis and Biological Evaluation of Hydrazide Desivatives as Diacylglycerol Acyltransferase-1 Inhibitors

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In mammals, diacylglycerol acyltransferase (DGAT) have two isoforms, DGAT-1 and DGAT-2. Although both isoforms are widely expressed and present at high levels in white adipose tissue, DGAT-1 is most highly expressed in the small intestine. DGAT-1 and DGAT-2 are two of the enzymes that are responsible for the main component of triglyceride (TG) synthesis in most organisms, and they have been studied in many eukaryotic organisms. Acyl-CoA:diacylglycerol acyltransferase-1 (DGAT-1) catalyzes the final committed step in the biosynthesis of triglycerides. Excessive accumulation of TG in human adipose and non-adipose tissues, however, is related to a variety of pathological conditions such as obesity, type 2 diabetes, coronary heart disease, hypertriglyceridemia and non-alcoholic fatty liver disease.In our search for novel DGAT-1 inhibitors, a series of hydrazide derivatives was synthesized and tested against DGAT-1 and 2, which resulted in novel DGAT-1 selective inhibitors with inhibition of triglyceride formation in HepG2 cells. Synthetic procedure and biological activity will be discussed in detail.

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Understanding of molecular mechanism of BLT1 and BLT 2 angonism/antagonism and selectivity

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Leukotriene B4, dihydroxy fatty acid formed from arachidonic acid by the 5-lipoxygenase pathway, is a potent chemoattractant of leukocytes, which are involved in various inflammatory diseases. The LTB4 receptor is a target for antiinflammatory drugs, and many antagonists of it have been developed and are being evaluated but none have yet been approved for clinical use. Two G-protein-coupled receptors for LTB4 have been identified. BLT1 is a high affinity receptor exclusively expressed in leukocytes, while BLT2 is a low affinity receptor expressed more extensively. Current studies on LTB4 receptors suggest the possibility of new clinical drugs being developed for the treatment of asthma, pancreatic cancer, arteriosclerosis and rheumatoid arthritis. To understand the molecular mechanism of BLT1 and BLT2, we constructed BLT1 and 2 homology models based on morphine receptor and performed docking studies for design of novel BLT2 selective antagonists. Based on these homology models, several derivatives were prepared and screened in BLT1 and 2 overexpressed CHO cells. Among the synthesized compounds, several compounds were found to be selective antagonists for BLT2. Representative BLT2 antagonists were tested in the murine model of asthma, in which airway wall thickness and airway obstruction were decreased by BLT2 antagonists and hypersensitivities of airway by methacholine were decreased by BLT antagonists. Our study may explain the molecular mechanism of BLT 1 and 2 agonistic/antagonistic effect as well as selectivity from the molecular modeling study. Furthermore, structure-activity relationship and in vivo studies of BLT2 selective antagonists warrant further biochemical study of BLT1 and 2 antagonism for the development of novel therapeutic agents targeting BLT2.

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Discovery of novel small molecules for the protection of mitochondria from hydrogen peroxide toxicity during ischemic stroke

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Stroke is the third leading cause of death and the major cause of long-term disability in the United States. It is known that under normal physiological conditions, the concentration of H2O2 in the cells remains low because of its detoxification by two enzymes called catalase and glutathione peroxidase.1 However, during ischemic stroke, the level of H2O2 is dramatically increased in the cells in spite of the presence of these two enzymes, which results in induction of oxidative stress and finally cell death.2 Recently, it has been reported that the major reason of cells death is due to the decrease of mitochondrial transmembrane potential (Δψm) by H2O2.3 In the present work, we present novel small molecules which protect the cells from H2O2 in case of pathological conditions like ischemic stroke and Parkinson disease by keeping the mitochondrial transmembrane potential high.

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Discovery of substituted pyridoxazine derivatives as novel c-Met kinase inhibitor

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Receptor tyrosine kinase (RTK) family is an attractive target for cancer therapy. c-Met kinase is a member of this family with its ligand, hepatocyte growth factor (HGF) or scatter factor (SF) which is crucial for normal mammalian development. c-Met is known to be over-expressed and mutated in a variety of human cancer types. c-Met is accountable proliferation, scattering, invasion, and metastasis of tumor cells. In an effort to search c-met kinase inhibitors, substituted pyridoxazine derivatives were synthesized and evaluated toward c-Met kinase inhibitory activity. Some of the compounds displayed excellent activity in vitro enzymatic and cell-based assay.

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Identification of Anti-oxidative, Whitening and Anti-inflammatory Constituents from Oreocnide fruticosa Branches

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제주대학교 화학과

In this study anti-oxidative, whitening and anti-inflammatory activities were examined on the extract from Oreocnide fruticosa branches and their biologically active constituents were identified. From repeated fractionation procedures, 7 compounds were isolated from Oreocnide fruticosa branches; friedelin (1), friedelanol (2), 5,7-dihydroxychromone (3), methyl vanillate (4), catechin (5), epi-catechin (6) and scopoletin (7). The structures of these compounds were confirmed by comparing their spectroscopic data to those in the literature. All of these compounds (1-7) were isolated for the first time from O. fruticosa. The isolated compounds were examined for anti-oxidative, whitening and anti-inflammatory activities. For the anti-oxidative activity test, the compounds 5 and 6 showed good DPPH radical scavenging activities with SC50 of 40.05 and 29.92 μM respectively, whose activities were comparable to a positive control vitamin C (SC50 46.23 μM). In addition, compounds 5, 6 and 7 showed good ABTS radical cation scavenging activity with SC50 of 7.56, 7.21, 64.04 μM respectively, showing comparable activity to vitamin C (SC50 31.32 μM). On the tyrosinase inhibition activity test, the compound 7 showed good inhibitory activity with IC50 111.80 μM, whose activities were more potent than a positive control arbutin (IC50 209.68 μM). For the anti-inflammatory activity test, the compound 7 showed inhibitory activity with 48.5% at 300 μM, without showing any cytotoxicity. Based on these results, O. fruticosa branches extract could be potentially applicable as cosmeceutical ingredient.

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Identification of Anti-oxidative and Anti-inflammatory Constituentsfrom the Branches of Corylus hallaisanensis

김성천 강지미 강다향 장형수 이남호*

제주대학교 화학과

Corylus hallaisanensis Nakai, a deciduous shrub growing in Jeju island, was investigated for anti-oxidative and anti-inflammatory activities. The dried C. hallaisanensis branches was extracted for 24 hour with 70% ethanol. The obtained extract was successively partitioned into n-hexane (Hex), ethyl acetate (EtOAc), n-butanol (BuOH) and water (H2O) fractions. Further phytochemical studies were conducted for the EtOAc fraction, which led to isolation of four constituents such as β-sitosterol (1), 3,3',4'-tri-O-methylellagic acid (2), carpinontriol A (3) and carpinontriol B (4). All of the compounds were isolated for the first time from this plant. On the studies of anti-oxidative activities for the isolated compounds, compounds 3 and 4 showed strong ABTS+ radical scavenging activities with SC50 of 19.3 and 12.9 μM respectively, whose activities were comparable to a positive control vitamin C (SC50 45.4 μM). On screening of anti-inflammatory activities, the compounds 2, 3, 4 showed considerable inhibition on the production of nitric oxide for the RAW 264.7 cell without showing cell toxicities. Based on these results, it is suggested that C. hallaisanensis branch extract could be potentially applicable in the cosmetical and/or pharmaceutical industries, especially as anti-oxidant and anti-inflammatory ingredient.

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Au-198 이 표지된 엽산-실리카 금 나노복합물질의 합성 및 평가

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실리카로 코팅된 금 나노복합물질에 화학물질로서 엽산을 결합하여 원자로에서 Au-197(n, r)Au-198 핵반응을 통해 방사성의약품으로서 기능 할 수 있을 것으로 보여 지며, 합성된 나노 복합물질은 분광학적 방법을 통해 분석하였다. 엽산과 암세포에 과발현된 엽산 수용체와의 결합을 통해서 방사화된 금에서 나오는 베타선으로 암 치료제로서 치료용 방사성의약품의 기능을 수행할 수 있다. In vitro, 합성된 나노복합물질로 마우스 대장암 세포인 CT-26 과 유방암 세포인 SK-BR-3 를 대상으로 세포 섭취도 실험을 진행한 결과, 15, 30, 60, 120 분에서 각각 CT-26 세포는 35%, 39%, 41%, 49%이며, SK-BR-3 에서는 32%, 38%, 40%, 48%로 시간이 지남에 따라 약물에 대한 세포 섭취도가 증가함을 확인 하였다. In vivo, CT-26 종양이 자란 balb/c 마우스로 나노복합물질의 생체내분포도를 측정한 결과 혈액대비 종양이 시간이 증가함에 따라 분포도가 120 분에서 약 2 배 이상 증가 하였다. 또한, 진단 및 치료를 같이 병행 할 수 있도록 합성된 나노 복합물질에 F-18 을 표지한 후 PET 이미지를 측정한 결과 암에 대한 진단제로서 이용 가능할 것으로 보여 진다. 이러한 연구 결과를 토대로, Au-198 나노복합물질이 암 치료제로서 동시에 F-18 이 표지된 나노복합물질로는 진단제로서 사용하여 양기능성 방사성의약품으로 사용 할 수 있을 것으로 기대된다.

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Novel 2-anilinoquinoline derivatives as sorafenib analogues: design, synthesis and in vitro antiproliferative activity

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A series of novel 2-anilinoquinolines has been designed and synthesized as sorafenib analogues. All the target compounds were evaluated for their antiproliferative activity against three cancer cell lines (MCF7, HCT116 and SKBR3) by MTT assay. Furthermore, five compounds were selected to be tested over a panel of 60 cancer cell lines at a single dose concentration of 10 uM at national cancer institute (NCI). Two compounds have showed promising mean growth inhibitions and were further tested at five-dose testing mode to determine their GI50, TGI and LC50 over the 60 cell lines. The data obtained revealed that compound 1j is the most potent and efficacious derivative with GI50 value of 0.356, 0.6, 0.66 and 0.678 uM against MDA-MB-468, UACC-62, A498 and SK-MEL-5 cell lines, respectively.

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Simultaneous Determination and Validation in Human Plasma by LC-MS/MS for Pharmacokinetics of Acetaminophen/Tramadol Combination Tablet

정영림

경기과학고등학교 화학생명과학부

A rapid, sensitive, and specific method for the simultaneous determination of acetaminophen and tramadol in human plasma, using acetaminophen-d4 and tramadol-d6 as internal standard, is described. Sample preparation involved a simple liquid-liquid extraction procedure. The extract was analyzed by high-performance liquid chromatography coupled to electrospray tandem mass spectrometry (LC-MS /MS). Chromatography was performed isocratically on a Hypersil gold C18 (2.1× 150 ㎜, 5 ㎛, Thermo) with acetonitrile and 10 mM ammonium acetate (pH 4.0) (50:50, v/v) as mobile phase. The instrument was set up in multiple reaction monitoring (MRM) mode; the transition m/z 152.1 → 110.1 was monitored for acetaminophen and the transition m/z 264.2 → 58.2 for tramadol. Calibration curves were linear over the range of 0.02～10 ug/mL for acetaminophen and 0.5～300 ng/mL for tramadol. The inter-run relative standard deviations were less than 6.37% for acetaminophen and 5.34% for tramadol. The intra-run relative standard deviations were less than 3.11% for acetaminophen and 2.47% for tramadol. The mean plasma extraction recovery to acetaminophen and tramadol were in the ranges of 71.54～77.24% and 91.82～98.39%. The developed assay method was applied to a pharmacokinetic study in healthy volunteers after oral administration of a new formulation acetaminophen/tramadol combination tablet.

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Role of Diversity Libraries of Korea Chemical Bank in Drug Discovery

김선우* 황순희* 이현규*

한국화학연구원 한국화합물은행

한국화합물은행은 신약연구와 관련하여 화합물 Library 를 활용하는 산?학?연 기관이 총체적으로 참여하는 형태로 운영되고 있으며. 현재 180 여개 기관에서 26 만종의 화합물을 기탁 받아 보관 관리하고 있다. 이렇게 확보한 화합물은 현재까지 220 개 산, 학. 연 기관에서 모두 525 종류의 작용점을 대상으로 대량약효검색(HTS or MTS)에 활용되어 Hit 를 대상으로 한 선도물질화 연구를 지원하고 있으며, HTS 후 도출된 Hit 평가 과정에서 Hit 화합물의 순도 및 물리화학적 물성평가, pharmacophore 검색을 통한 SAR 자료, 작용점에 대한 최근 연구개발 동향 및 Hit 골격과의 연관성, Pre-ADME 검색을 통한 선도물질성, 3D-QSAR 결과 등을 관련기관에 제공하고 있다. 아울러 Hit 발생 빈도가 높은 화합물 골격에 대한 조사를 통하여 false positive 에 대한 일반적 정보를 제공하여 선도물질개발을 위한 Hit 평가를 좀 더 효율적으로 진행할 수 있도록 하고 있다. 그 결과 독창적인 골격을 지닌 Hit 가 다량 도출되고 있으며, 좀 더 효율적인 HTS 를 위해서 Focused library(Clinical Collection, Kinase, Fragment 등)를 구축하여 약효시험기관에 제공하고자 하며, 이러한 "Hit to Lead"와 화합물은행의 역할에 대하여 발표하고자 한다.

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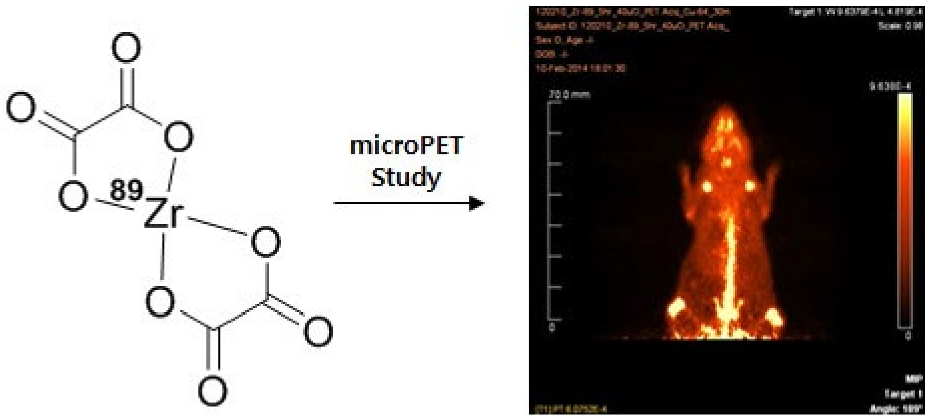
Medical Application of Zr-89 Oxalate for PET Radiopharmaceutical

이지웅 박지애[1] 신운철[2] 이교철[3] 안광일[4,*] 김정영[3,*]

고려대학교 보건과학 [1]한국원자력의학원 분자영상연구부 핵의학연구팀 [2]연세대학교 의공학과 [3]한국원자력의학원 방사성의약품연구팀 [4]한국원자력의학원 방사성의약품 개발실

Objective: Positron-emitted Zr-89 (Zirconium, half-life 3.27 days) in clinic has recently been reported to be particularly effective at PET imaging. Such Zr-89 depends on a good bifunctional chelator and proper biomolecule (peptides, antibody, etc.) for specific binding in cell. The aim of our study, thus, was to widen the use of Zr-89 in Korean clinic with development of PET technology. Material & Method: Zr-89 was generated by nuclear reaction of 50 MeV cyclotron (Scantronix co.) in KIRAMS, which was used as target material of yttrium foil. The nuclear reaction was carried out Y-89(p,n)Zr-89 under irradiation of proton beam (20 μA, 18 MeV) for 2 hours. The purification of Zr-89 was performed with a specific Sep-PaK column (hydroxamate resin). On this column, Zr-89 oxalate was rapidly prepared as high radiochemical purity. Result: Zr-89 oxalate was easily prepared by short column, and the radiochemical purity was over 99%. The radiochemical yield of product was obtained as radioactive solution of 9-13 mCi in hydrochloric acid (1 mL, 1 M). Zr-89 was showed the specific gamma-energy of both 511 and 909 KeV as reported previously. Zr-89 oxalate, thus, was successfully exhibited good PET imaging of bone marrow in mouse. Zr-89 was further studied the ability of PET imaging using phantom and microPET scanner.Conclusion: The development of Zr-89 oxalate may be extended to the studies of new radiotracer for PET molecular imaging.


O
O
O
O
89Zr
O
O
O
O
microPET
Study
10-Feb-2014 18:01:30
70.0 mm
0
0
MIP
Target 1

일시: 2014년 4월 16~18일(수~금) 3일간
장소: 일산KINTEX
발표코드: **MEDI.P-898**
발표분야: 의약화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Development and Optimization of a Fluorescence Polarization Assay for PIM Kinases

이성호 이진호 **HONG VICTOR SUKBONG***

계명대학교 화학과

Pim proteins consisting of Pim1, 2, and 3 are a family of serine/threonine kinases that regulate fundamental cellular responses such as cell growth, differentiation and apoptosis. Deregulation of the Pim kinases has been linked to a wide variety of hematological and solid tumors. Thus, all three Pim kinases have been studied as promising targets for anticancer therapy. Here, we report on the development and optimization of an immobilized metal ion affinity-based fluorescence polarization (IMAP) method for Pim kinases. In this homogeneous 384-well assay method, FITC-labeled phosphopeptides are captured on modified nanoparticles through interactions with immobilized trivalent metals, yielding high polarization values. The IMAP assay for Pim kinases not only allows for high-throughput screening but also facilitate the identification of novel Pim inhibitors for drug development.

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장소: 일산KINTEX
발표코드: **MEDI.P-899**
발표분야: 의약화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Discovery of substituted hydrazinone pyrimidine derivatives as novel c-Met kinase inhibitor

정희정* 조성윤 하재두 김은영[1] 강승태[1]

한국화학연구원 난치성질환치료제연구센터 [1]성균관대학교 화학과

Receptor tyrosine kinase (RTK) family is an attractive target for cancer therapy.? C-Met kinase is a member of this family with its ligand, hepatocyte growth factor (HGF) or scatter factor (SF) which is crucial for normal mammalian development.? c-Met is known to be over-expressed and mutated in a variety of human cancer types.? c-Met is accountable proliferation, scattering, invasion, and metastasis of tumor cells. In an effort to search of c-met kinase inhibitors, substituted hydrazinone pyrimidine derivatives were synthesized and evaluated toward c-met kinase inhibitory activity. Some of the compounds showed moderate activity in vitro enzymatic and cell-based assay.

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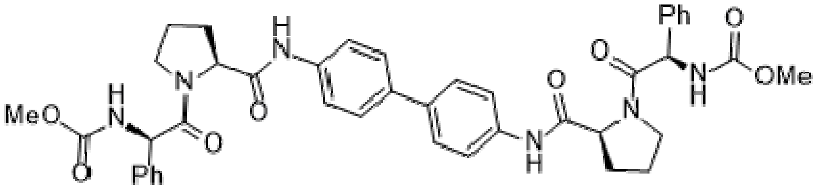
발표분야: 의약화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Potent Hepatitis C Virus NS5A Inhibitors: Discovery of BMK-20113

배일학 김병문*

서울대학교 화학부

Hepatitis C virus (HCV) belongs to the hepacivirus genus in the Flaviviridae family as a single-positive-stranded RNA virus and its infection often leads to serious diseases such as liver cirrhosis and eventually to hepatocellular carcinoma. HCV RNA consists of structural and nonstructural proteins. Especially, several non-structural proteins (NS2, NS3, NS4A, NS4B, NS5A and NS5B) involved in the reproduction of HCV are of great importance for new therapeutic target identification. However, current standard of anti-viral therapy has been the combination of pegylated interferon-α with ribavirin (Peg-IFN/RBV), until a recent addition of the HCV protease inhibitors such as Telaprevir and Boceprevir. Therefore development of effective anti-HCV drug candidates is urgently needed. Here we report the discovery of a series of HCV NS5A inhibitors based on the benzidine prolinamide skeleton. Taking a simple synthetic route, we developed a novel inhibitor structure, which allows easy modification, and through optimization of the capping groups, we identified BMK-20113 with highly potent anti-HCV activity. BMK-20113 is nontoxic and is anticipated to be an effective HCV drug candidate.



Type 2a: EC_{50} = 0.26 nM, G-1b: EC_{50} = 0.028 nM

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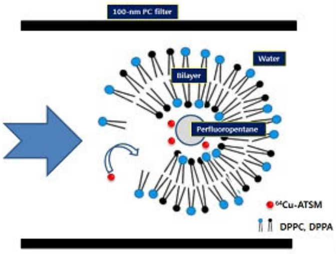
장소: 일산KINTEX
발표코드: **MEDI.P-901**
발표분야: 의약화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

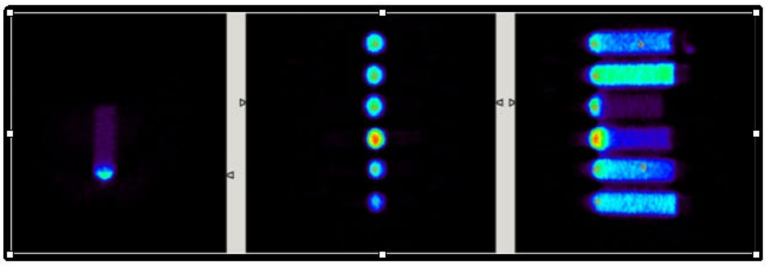
Multimodal Imaging Agent for Ultrasound and PET: Development of Liposome encapsulated [Cu-64]ATSM and Perfluorocarbon

신운철 이지웅[1] 박지애[2] 안광일[3] 이교철[4] 김정영[4,*]

연세대학교 의공학과 [1]고려대학교 보건과학 [2]한국원자력의학원 분자영상연구부 핵의학연구팀 [3]한국원자력의학원 방사성의약품 개발실 [4]한국원자력의학원 방사성의약품연구팀

Object: Contrast agent studies have been reported recently in feasibility of multifunctionl nanoparticles for multimodal imaging. The purpose of this study is to develop a specific liposome of nano-bubbles incoporating Cu-64 ATSM for PET and ultrasound imaging. Methods: Ultrasound contrast agent (UCA) was fabricated by perfluoropentane(PP) with liposome solution consisting of DPPC and DPPA (10 : 1, molar ratio). At the same time, Cu-64 ATSM was synthesized with Cu-64 dichloride and ATSM, which inserted into phospholipids bilayer by mini-extruder (4 ml/min, 26°C). The size of liposome, including perfluorocarbon and Cu-64 ATSM, was controlled by extrusion through 100 nm polycarbonate filter. The PET image was obtained by a small animal PET/CT scanner (InveonTM, Siemens). The acquired PET image was evaluated ROI using AMIDE image data program after reconstruction by the OSEM 2D algorithm with the FORE method. Ultrasound images were obtained by ultrasound image scanner (Sonoace Pico, Medison) using 5 MHz linear probe with B mode in degassed water tank. The acquired utrasound image was evaluated by the average brightness of ROI. Result: The mean activity of only Cu-64 ATSM and roll-mixed PP-UCA were uniformly observed in whole area, respectively. However, the mean activity of PP-UCA produced by vial-mixer and 100 nm air-UCA were increased to 163% and 146% in the lower area than other area, respectively. ROI mean Activity of 100 nm PP-UCA was increased to 280% in lower area than only Cu-64 ATSM. The product was also showed strongly contrast-enhanced ultrasound images after approximately 10 min at 40°C. Conclusion: Liposome (100 nm, size) could put in Cu-64 ATSM and perfluorocarbon, which was showed the potential multimodal imaging agent of ultrasound and PET.


100-nm PC filter
Water
Bilayer
Perfluoropentane
⁶⁴Cu-ATSM
DPPC, DPPA



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장소: 일산KINTEX
발표코드: **MEDI.P-902**
발표분야: 의약화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

화합물분야 국가 연구성과물 기탁제

황순희 김선우 최중권 이주연 이현규*

한국화학연구원 한국화합물은행

정부는 국가연구개발사업 성과물의 체계적인 관리와 공동 활용을 위하여 국가연구개발사업 8 대 연구성과물 전담기관을 지정하여 운영하고 있다. 한국화합물은행(www.chembank.org)은 미래창조과학부로부터 국가연구개발사업 성과물 중 화합물분야의 관리 · 유통 전담기관으로 지정되어 있으며 (미래창조과학부 고시 제 2013-128 호), 국가연구개발사업 수행을 통해 창출된 화합물 및 관련 정보에 관한 관리 · 유통체계구축 및 운영업무를 수행하고 있다. 또한 「국가연구개발사업의 관리 등에 관한 규정」 제 25 조 제 13 항에 따라 국가연구개발사업 수행을 통해 창출된 모든 화합물은 의무적으로 화합물분야의 관리 · 유통 전담기관인 한국화합물은행에 기탁되어야 한다. 한국화합물은행은 화합물 기탁자에게 기탁필증을 발급하고 있으며, 기탁된 화합물 현황정보는 매년 NTIS(국가과학기술지식정보서비스, www.ntis.go.kr)에 등록되고 있다.한국화합물은행에서는 연구성과물(화합물)로 기탁된 화합물과 관련정보를 체계적으로 관리하고 스크리닝용 플레이트를 생성하여 연 평균 40 여건 다양한 질병 타겟에 20 여만개 이상의 화합물을 제공하여 고효율약효검색(HTS) 활용을 지원하고 있으며, 축적된 화합물 구조정보 및 약효검색 결과정보를 가공, 분석한 화합물 구조-약효관련 정보시스템을 구축중에 있다.한국화합물은행은 잠재적 무한 가치를 갖는 화합물들을 범국가적으로 수집하고 통합관리하며, 고효율 약효검색 등에 공동 활용함으로써 글로벌 신약개발연구 및 BT 연구를 지원하는 국가 핵심인프라 구축에 기여하고 있다.

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

An effective route for size- and morphology-controlled synthesis of platinum nanomaterials in an aqueous solution via proton beam irradiation

이윤지 송재희*

순천대학교 화학과

We present a facile one-pot synthetic route for the production of platinum nanomaterials via a simple proton beam irradiation process at room temperature. Hexadecyltrimethylammonium bromide(CTAB) was used as a stabilizing reagent for the preparation of platinum nanomaterials. Size-and shape-controlled platinum nanostructures were prepared in an aqueous phase-based solution without the addition of any harsh reductants. We observed that the size and morphology of platinum nanoparticles were controlled by controlling the proton beam current and the duration of irradiation. It was also observed that the addition of isopropyl alcohol to the reaction mixture played a vital role for the morphology controlled synthesis of platinum nanomaterials. The characterization was done by using UV-Vis absorption spectroscopy, TEM, and EDS analyses.

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

Reversible Layer-by-Layer Deposition on Solid Substrates Inspired by Mussel Byssus Cuticle

김수엽 강성민*

부경대학교 해양바이오신소재학과

The protective coating on mussel (Mytilus galloprovincialis) byssus has attracted considerable research interest because of its excellent mechanical properties such as hardness and extensibility. These special properties are known to be highly related with specific interactions between mussel foot protein-1 and metal ions. In particular, the complexation between catechols in mfp-1 and iron(III) has been identified as a key interaction. This finding has given opportunities for pursuing promising applications. Herein, we report that emulating the properties of the mussel byssus cuticle provides an important platform for developing reversible layer-by-layer (LbL) deposition, an advanced technique for surface modification. LbL films were constructed on solid substrates by sequential immersion of substrates into solutions containing iron(III) and catecholic compounds. The thickness of the LbL films was effectively controlled by increasing the immersion steps, and the reversibility of the LbL deposition was demonstrated by addition of a chelating agent.

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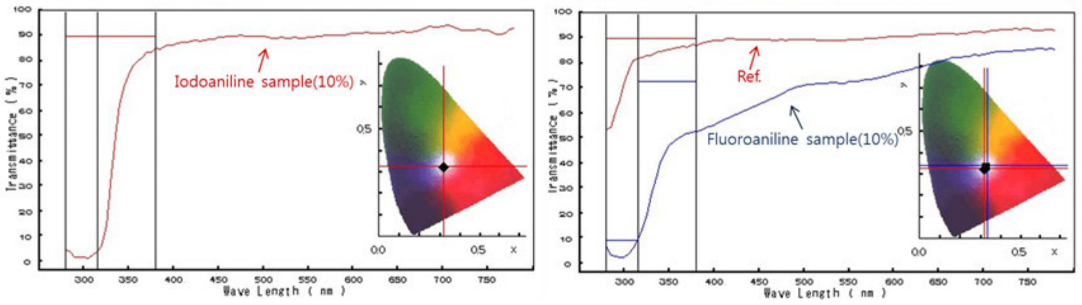
발표분야: 재료화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Preparation and Characterization of Ophthalmic Polymer including Iodine and Fluorine substituted Aniline

노정원 김동현 성아영*

세한대학교 안경광학과

Recently, many eye disease associated with ultraviolet radiation were reported. In this study, the UV-block ophthalmic lens using iodoine, fluorine-substituted aniline group were manufactured and the physical properties of copolymerized materials were measured. The basic hydrogel ophthalmic lens material with addition of 3-Iodoaniline and 4-Fluoroaniline respectively were polymerized and the hydrogel ophthalmic lens was manufactured by cast mould method. The ophthalmic lenses were stored in a 0.9% NaCl normal saline for 24 hrs. The measurement of the physical properties of the copolymerized polymer with addition of Iodoaniline showed that the refractive index increased and the water content decreased as the ratio of additive increased. Also, the polymer including Fluoroaniline, the average value of refractive index decreased and the water content increased as the ratio of additive increased. In the case of Iodoaniline sample(10%), the optical transmittance measurement showed the UV-B transmittance of 2.4%, UV-A transmittance of 48.2% and visible transmittance 90.0%. Also, in the case of Fluoroaniline sample(10%), the optical transmittance of UV-B, UV-A and visible transmittance were measured 9.0%, 36.0% and 75.0%, respectively.



(a) Iodoaniline

(b) Ref. and Fluoroaniline

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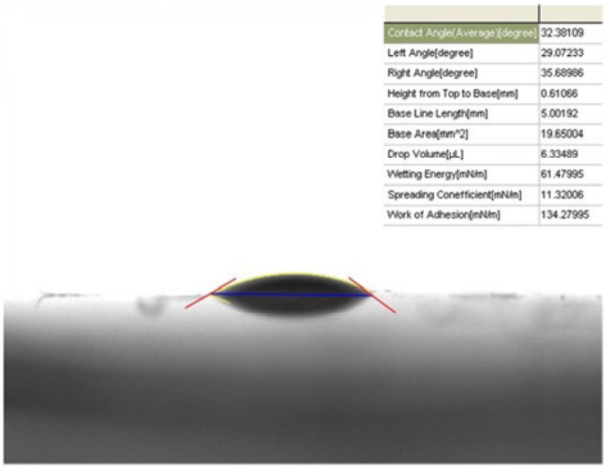
발표분야: 재료화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Influence of wetting materials on hydrogel ophthalmic lens

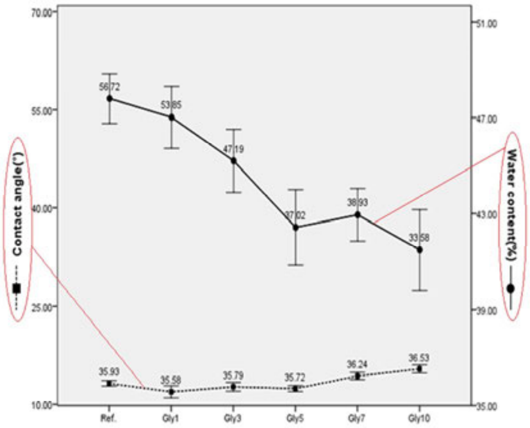
이민제 성아영*

세한대학교 안경광학과

The physical and optical characteristics of hydrophilic contact lens polymerized with addition of glycerin and PVP(polyvinylpyrrolidone) in the basic hydrogel contact lens material were evaluated. Glycerin and PVP with the cross-linker EGDMA(ethylene glycol dimethacrylate), HEMA(2-hydroxyethyl methacrylate) and the initiator AIBN(azobisisobutyronitrile) were used for thermal copolymerization. The cast mould method was used to fabricate the hydrogel contact lens. The mixture was heated at 100℃ for 40 mins to produce the hydrogel lens. Measurement of the physical characteristics of the copolymerized material showed the refractive index of 1.4382~1.4288, tensile strength of 0.3446~2542kgf, water content of 36.15~41.79%, and contact angle of 59.93~47.08°. And also, the physical characteristics of the copolymerized material including glycerin showed the refractive index of 1.4330~1.4328, tensile strength of 0.2974~0.2854kgf, water content of 35.58~36.53%, and contact angle of 53.85~33.58˚. It is judged that the copolymers is suitable for conventional lens with high wettability. However, glycerin minimized the changes of water content and refractive index at the same time, increased the wettability of the hydrogel lens materials.



Contact Angle(Average)[degree]	32.38109
Left Angle[degree]	29.07233
Right Angle[degree]	35.68986
Height from Top to Base[mm]	0.61066
Base Line Length[mm]	5.00192
Base Area[mm^2]	19.65004
Drop Volume[μL]	6.33489
Wetting Energy[mN/m]	61.47995
Spreading Conefficient[mN/m]	11.32006
Work of Adhesion[mN/m]	134.27995



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발표코드: **MAT.P-907**
발표분야: 재료화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Ultrasound-assisted Polyol Synthesis of Pt Nanoparticles on the various 2-Dimensional Nanomaterials and Their Electrocatalytic Properties for Methanol Oxidation

김성복 권영욱*

성균관대학교 화학과

In this study, we report the ultrasound-assisted polyol synthesis (UPS) of Pt nanoparticles (NPs) on various 2-dimensional nanomaterials (graphene, graphitic carbon nitride and molybdenum disulfide) and their electrocatalytic properties for methanol oxidation reaction (MOR). We expected that Pt NPs is formed by galvanic replacement between Pt^{2+} and Mn^0 in the ethylene glycol media. Therefore, Mn seed formed from manganese acetylacetonate is significant intermediates to make uniform and well-dispersed Pt NPs on 2-dimensional nanomaterials. Based on structural analysis results, we confirmed that every samples have uniform particle size (2~3 nm) and high dispersion of Pt NPs on each 2-dimensional nanomaterials. Electrochemical properties of samples are investigated by using rotating disk electrode (RDE) measurements. Interestingly, we observed that MOR activity of Pt NPs could be affected by interaction with 2-dimensional nanomaterials. Among the three types of samples, Pt/MoS_2 showed the higher MOR current and CO-tolerance than other samples due to strong interaction between Pt and MoS_2.

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

High-aspect-ratio silicon microwire arrays by metal-assisted chemical etching for photovoltaic applications

엄한돈 황인찬 서관용[1,*]

울산과학기술대학교(UNIST) 에너지공학과 [1]울산과학기술대학교(UNIST) 친환경에너지공학부

Vertically aligned silicon microwire (MW) arrays have been extensively investigated as a means for developing highly efficient and low cost solar cells. Silicon surface patterned with the MW arrays leads to broadband antireflection as well as enhanced light trapping efficiency. Vertically-aligned MWs can be fabricated by several methods, such as vapor-liquid-solid (VLS), reactive ion etching (RIE), and metal-assisted chemical etching (MACE). Among them, owing to the low cost and wafer-scale fabrication, MACE is an attractive method to fabricate Si MWs. However, the detailed mechanism of Si MW etching using a metal thin film as a catalyst is still unclear. Here, we present a systematic study of MACE to fabricate Si MWs. Several models on efficient redox reactions of reactants with silicon though the metal catalyst were studied by controlling MACE parameters, such as the thickness and morphology of metal thin film and electrolyte concentration (HF and H_2O_2). As a result, by optimizing MACE conditions, we successfully fabricated high-quality Si MWs with lengths up to 17 μm. The minority carrier lifetime of these MWs, measured by the microwave photoconductive decay, is higher than that of MWs etched by DRIE process. The MACE method of high-quality Si MWs would offer opportunities to develop cost-effective, highly efficient solar cells.

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For assessment of the safety of Nano-contrast agent the physical and chemical characterization of the test protocol establish

송미령 정민숙 박수진 김준성*

(주)바이테리얼즈 부설연구소

Nano-contrast is currently commercialized in early stages of development, and the actual uthentication / use insufficient. Recently, however, a contrast effect more than two multimodal nanoprobe has been developed, utilizing nano-nano sensor contrast, Drug delivery, treatment of disease detection, and a variety of applications in nanobiotechnology research is actively being utilized in the situation. In this study, the establish testing protocol for the safety evaluation of nano- contrast agents and candidate substance.Candidate materials and technology for the first nano-contrast agents and the status of current research is investigation. Nano-Contrast examined in this current analysis of the physical and chemical characteristics of the test protocol provided.

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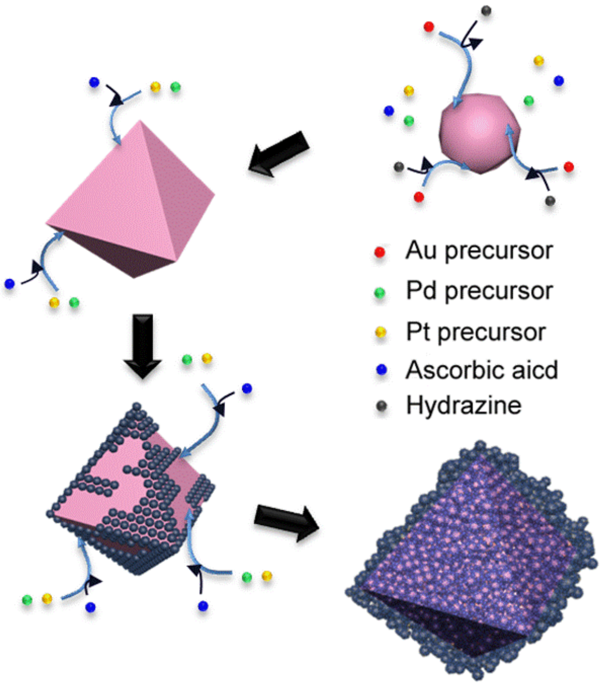
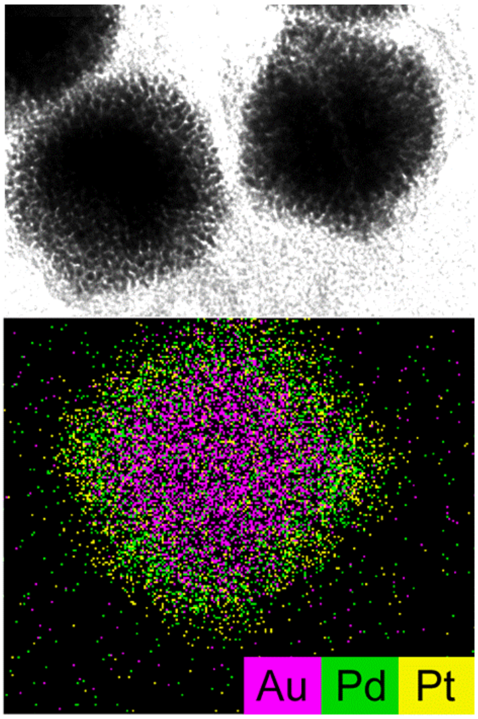
One-Pot Synthesis of Trimetallic Au@PdPt Core-Shell Nanoparticles with High Catalytic Performance

강신욱 한상우*

한국과학기술원(KAIST) 화학과

The development of an efficient synthesis method to produce multi-metallic nanoparticles (NPs) with a desirable structure is strongly required to clarify the structure-composition-property relationship of NPs and to investigate their possible applications. However, the controlled synthesis of NPs consisting of multiple ($n \geq 3$) noble metal components has been relatively unexplored in comparison to bimetallic NPs. In the present work, we have demonstrated a facile one-pot aqueous approach for the controlled synthesis of trimetallic Au@PdPt core-shell NPs with a well-defined octahedral Au core and a highly-crystalline dendritic Pd-Pt alloy shell (Au_{oct}@PdPt NPs). The simultaneous reduction of multiple metal precursors with dual reducing agents, namely, ascorbic acid and hydrazine, gave a fine control over the nucleation and growth kinetics of NPs, resulting in the formation of novel Au_{oct}@PdPt NPs. The prepared NPs showed excellent catalytic performance for methanol electrooxidation, which can be attributed to their optimized binding strength toward adsorbate molecules due to the improved charge transfer between core and shell of the NPs. The present strategy can offer a convenient and valuable way to fabricate multi-component nanostructures with desired structures and functions.


Au precursor
Pd precursor
Pt precursor
Ascorbic aicd
Hydrazine


Au
Pd
Pt

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Ionic conductivities of defect perovskites $\mathbf{Sr_{0.73}Li_{0.27}Ta_{0.73}O_{1.81}N_{0.58}}$ and $\mathbf{Sr_{0.7}Li_{0.3}Ta_{0.7}O_{2.6}}$

김정미 김영일*

영남대학교 화학과

Ammonolytic heating of the mixture of (1-x)$Sr_2Ta_2O_7$ and xLi_2CO_3 leads to perovskite phases with the general formula $Sr_{1-x}Li_xTa_{1-x}O_{3.5-3x-3y}$ N_{2y}which, on further heating in air, transforms to oxide $Sr_{1-x}Li_xTa_{1-x}O_{3.5-3x}$. The defective lattice structure of above phases gives implication to the ionic conductivity, and we measured the transport properties of $Sr_{0.73}Li_{0.27}Ta_{0.73}O_{1.81}N_{0.58}$ and $Sr_{0.73}Li_{0.27}Ta_{0.73}O_{2.6}$ by employing ac impedance spectroscopy. The equivalent circuit analysis of the measured impedance spectra indicated that $Sr_{0.73}Li_{0.27}Ta_{0.73}O_{2.6}$ has ionic conductivity (σ_{ion}) of 10^{-9} ~ 10^{-5} in the temperature range 300-900 K. Interestingly, σ_{ion} of $Sr_{0.73}Li_{0.27}Ta_{0.73}O_{2.6}$ showed a minimum at ?440 K, implying the mixed conduction from proton and Li^+. The ionic conductivity of $Sr_{0.73}Li_{0.27}Ta_{0.73}O_{1.81}N_{0.58}$was lower than that of $Sr_{0.73}Li_{0.27}Ta_{0.73}O_{2.6}$ by an order of ? 2.

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Fabrication of Superhydrophobic Surface on a Cellulose-based Material via Chemical Modification

황지수 안용현*

단국대학교 화학과

Superhydrophobic surfaces are highly hydrophobic; that is, they are extremely difficult to wet and have contact angles (CA) of greater than 150°. Superhydrophobicity is a fascinating surface property of wide application, for instance, to develop coatings for automobile windows, clothes and to separate oil and water mixture, etc. Superhydrophobicity surface is fabricated by forming a micro-/nanoscale structure on a surface and coating the surface with a low surface energy material. Typically, cotton fibers are interwoven with cellulose fibers, which contain numerous surface hydroxyl groups, so that resulting cotton fabric is superhydrophilic and highly wettable. The superhydrophobic cotton fabric which had been fatty acid modified have applied to separate oil and water mixture. The formation of superhydrophobic surface on the cotton fabric involved a chemical reaction. The surface hydroxyl groups of the cotton fabric underwent esterification with stearic acid in the presence of DCC and catalytic amount of DMAP in methylene chloride . The WCA of the untreated cotton fabric was 0o because of the abundance of surface hydroxyl groups and the resulting hydrophilicity. On the other hand, the the chemically modified cotton fabric became superhydrophobic(WCA of 150o) because of the esterification of the hydroxyl groups with stearic acid. We confirmed the successful esterification reaction and the formation of fatty ester linkages using XPS and FT-IR.

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Thermal Oxidation of MoS_2 and MoS_2/Ag

이소람 김유혁*

단국대학교 자연과학대학 화학과

Orthorhombic molybdenum trioxide (α-MoO_3) have been synthesized by a thermal reaction in oxygen environment of MoS_2 at 500 ^{0}C. Morphological changes of MoO_3 from 500 ^{o}C to 900 ^{o}C were investigated with X-ray powder diffraction (XRD) and scanning electron micrscopy (SEM). Interestingly, the strong diffraction peaks of (020), (040) and (060) planes at 800 ^{o}C reveal a highly anisotropic growth of the oxides with a layered crystal structure. On the other hand, in the presence of crystalline Ag prepared by reduction of $AgNO_3$ with $NaBH_4$ the thermal reaction of MoS_2 produced silver molybdate (Ag_2MoO_4) as main product.

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Preparation of Exfoliated Ag-Laponite Nanocomposites Through a Freeze-Drying of Laponite Sols

남정원 김유혁*

단국대학교 자연과학대학 화학과

This work reports on Ag nanoparticles-laponite composites prepared by a freeze-drying method from resulting Ag nanoparticle sols. The adsorption behavior of Ag nanoparticles into laponite is investigated. Intensities of absorption peaks due to Ag nanoparticles in laponite at about 405 nm increased with the increase of silver nitrate concentration. Ag nanoparticles in laponite in TEM pictures show a mixture of smaller and larger particles about 3~8 nm and 10~20 nm, respectively. Ag-laponite nanocomposites were prepared through a freeze-drying method of lapnite sol containing Ag nanoparticles. The sizes of Ag nanoparticles calculated by XRD data and observed from TEM experiments are too large for nanoparticles to be accommodated between the layers of the clay, which was calculated as ~ 0.46 nm. This suggests that the intercalation of nanoparticles is excluded and a considerable amount of Ag nanoparticles are likely to be deposited on the external surfaces of the clay. With high nanosilver concentrations, most of the d_{001} reflections and peaks characteristic of laponite disappeared, suggesting that laponite is exfoliated after the formation of large Ag particles. The XRD patterns of laponite decomposition for the thermally treated samples confirms the presence of laponites.

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Synthesis, characterization, and photocatalytic analysis of GO-TiO_2

김성필 최현철*

전남대학교 화학과

The nature of carbon-based supports is critical for the electrocatalytic activity, dispersion, stability, mass transfer kinetics at the electrode surface, and electric conductivity of a catalyst. Graphene is a promising carbon candidate because of its extremely large specific surface area, high electrical conductivity, good chemical and thermal stability, which is widely used to support catalysts like metals, metal oxides. In this study, we prepared GO-TiO_2 by treating thiol groups on graphene surfaces. The obtained GO-TiO_2 were characterized by using X-ray photoelectron spectra (XPS), X-ray diffraction (XRD) and transmission electron microscopy (TEM). The photoactivity of the prepared materials was evaluated by the conversion of methylene blue in aqueous solution under UV irradiation.

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Synthesis of Thiol-Functionalized Silver Nanoparticles Using Modified One-Phase Method

홍지영 정민혜 이소람 김유혁*

단국대학교 자연과학대학 화학과

One-phase synthesis for thiol-functionalized silver nanoparticles has been modified by changing the order of addition of reducing agent to give significantly larger (~20 nm) silver nanoparticles. This method is advantageous to isolate large amount of clean silver nanoparticles. The products are characterized by Uv-vis spectra, X-ray powder diffraction (XRD), transmission electron microscopy (TEM), ^{1}H NMR. In addition to this, the dependence of Ag^+ : R-SH ratios on giving thiol-functionalized silver nanoparticles and layered siver thiolated complexes was investigated.

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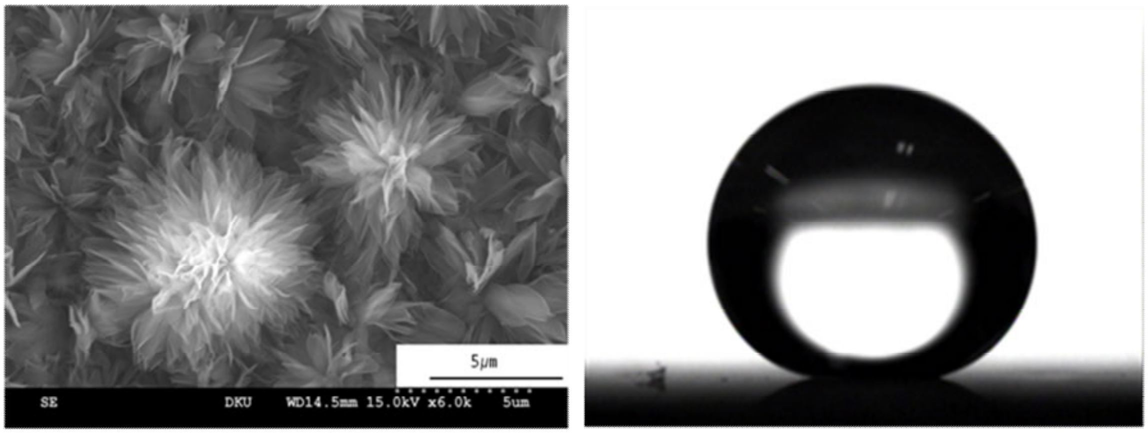
Facile Fabrication of Metal Surfaces Having Superhydrophobic Property

김영아 안용현*

단국대학교 화학과

Superhydrophobic surfaces have important technical applications ranging from self-cleaning window glasses, paints, and fabrics to anti-corrosion surfaces. To fabricate a superhydrophobic surface, two factors must be combined. One is the creation of nano-/micro- rough structures on the surface, and the other is coating with low surface materials such as long chain fatty acid, fluorinated alkyl silanes to lower the surface energy of the hierarchical surface of the solid material. In this experiments, we try to fabricate superhydrophobic surfaces on various substrates, such as glass, magnesium, copper plate, and aluminium plate. We fabricate a superhydrophobic surface by dipping metal plates in a solution of fluorinated alkyl silane and alkylphosphonic acid in ethanol. In the presence of propylphosphonic acid, HFTHTMS is polymerized and then deposited on the surface during the immersion period. Many flower-like structures were formed on the magnesium surface after at least 10min of immersion. In copper plate, plate-shaped structures were formed after 12h of immersion. But, superhydrophobic surfaces not observed on the aluminium and glass. We guess that the problem is due to low adhesion between the substrate and polysiloxane. Taking inspiration from the adhesion of marine mussels, we try to pretreatment the surface with dopamine. Dopamine and its catecholic derivatives are able to undergo oxidative polymerization in the presence of oxygen as an oxidant under alkaline conditions.


5μm
SE
DKU
WD14.5mm 15.0kV x6.0k
5um

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Cation effects on the properties of struvite cystals

이슬기 최현철*

전남대학교 화학과

Nitrogen and phosphorus in wastewaters are a burning environmental issue of the present world. Struvite($MgNH_4PO_4 \cdot 6H_2O$) is a white crystalline material and has obtained interest as a route to phosphorus recuperation. But struvite precipitation is influenced by many factors including concentration of Mg^{2+}, NH_4^+ and PO_4^{3-} ions, pH, and impurity cations (K^+, Ca^{2+} and Al^{3+} etc). Recently, struvite is also considered as a potentially marketable product as an alternative fertiliser. The objective of this study conducted on the recovery of phosphorus and nitrogen from distilled waters through struvite crystallization. In this study, the cation effects on struvite precipitation were evaluated by scanning electron microscopy (SEM), X-ray diffraction (XRD), energy dispersive spectrometry (EDS), and thermogravimetric analysis (TGA).

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Photocatalytic properties of CNT-SnO_2

김성필 최현철*

전남대학교 화학과

Recently, photocatalysis has played an important role in the environmental procedures such as air purification, water disinfection and purification. Among them,Tin Oxide (SnO_2) has been used as a photocatalysis for degradation of a wide variety of environmental pollutants due to its advantages like low cost, easy production, and compact size etc. The photocatalytic efficiency of SnO_2 mainly depends on high specific surface area of SnO_2 particles, crystal structure, particle size and porosity. One of the methods to improve the photocatalytic efficiency is to increase the surface area of the catalyst. In this study, We was manufactured CNT-SnO_2 using multi-walled carbon nanotubes as a supporting material and tin (Ⅱ) chloride as tin source. The morphology and structure of CNT-SnO_2 are also examined by transmission electron microscopy (TEM), X-ray diffraction (XRD) and X-ray photoelectron spectroscopy (XPS). The photoactivity of the manufactured materials was estimated by the conversion of methyl orange in aqueous solution under UV irradiation.

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Electrochemical oxidation of formalde on nanoparticles decorated multi-walled carbon nanotubes

이슬기 최현철*

전남대학교 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. 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, Samples were prepared using thiolated CNT by conventional oxidation method. The obtained sample were characterized using various analytical techniques such as SEM, TEM and XPS. Electrochemical oxidation of formalde on these catalysts are also investigated via cyclic voltammetric measurement. The results imply that the metal nanoparticles decorated CNTs exhibit a better activity than the compercial Pt catalysts.

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Structure Evolution of Asymmetric Molecule With Tetrathiafulvalene Moiety

<u>임푸른</u> 이명훈[1] 정광운[2,*]

전북대학교 고분자.나노공학과 [1]전북대학교 고분자나노공학과 [2]전북대학교 고분자.나노 공학과

An asymmetric molecule (asym-TTF) containing the tetrathiafulvalene was newly synthesized to control their molecular packing structure and morphology on the various length scale. The crystal structure was identified to be a monoclinic unit cell from the 2D WAXD pattern of the oriented asym-TTF. Moreover, the self-assembled ribbons aggregated themselves to form fibrous hierarchical structures with different diameters in the micrometer length scale and their structure is confirmed by utilizing TEM, AFM, and POM. During the crystallization process, generated unequable surface stresses lead to the scrolled and helical structures. This work was mainly supported by the Human Resource Training Project for Regional Innovation, Basic Science Research Program (2013R1A1A2007238), and BK21 PLUS Program, Korea.

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Preparation of graphite oxide/metal?organic framework (MIL-101) and adsorptive denitrogenation of model fuels with the composite

imteaz ahmed 정성화*

경북대학교 화학과

A porous metal?organic framework (MOF), MIL-101 (Cr-benzenedicarboxylate), was synthesized in the presence of graphite oxide (GO) to produce GO/MIL-101 composites. The porosity of the composites increased remarkably in the presence of a small amount of GO (

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Adsorptive removal of naproxen and clofibric acid over a metal-organic framework MIL-101 functionalized with acidic and basic groups

HASAN ZUBAIR 정성화[1,*]

경북대학교 대학원 화학과 [1]경북대학교 화학과

Adsorption of naproxen and clofibric acid, two typical PPCPs (pharmaceuticals and personal care products) has been studied with virgin and modified MIL-101s, one of the typical metal-organic frameworks (MOFs) [1]. Aminomethanesulfonic acid (AMSA) and ethylenediamine (ED) were used to coordinate (using the common -NH2 group) on coordinatively unsaturated sites (CUSs) or open metal sites of the MOF to generate an acidic (-SO3H) group and basic (-NH2) group, respectively. The highest removal efficiency was observed with ED-MIL-101 both for the adsorption rate and adsorption capacity. On the contrary, the performance of the acidic AMSA-MIL-101 was very poor. Therefore, the adsorption mechanism may be explained with an acid-base interaction between the PPCPs and the adsorbents. The effect of pH on the adsorption of naproxen also supports this acid-base interaction. Moreover, a functionalized basic MOF (with -NH2) can be regenerated by simple washing with ethanol and is reusable up to at least the third run with little change in the performance along with a high adsorption capacity and rapid adsorption which is important for commercial applications. Reference[1] Z. Hasan, E.J. Choi, S.H. Jhung, Chem. Eng. J.2013, 219, 537?544

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Effect of Post Heat-treatment on Fe, N doped Ordered Mesoporous Carbon Materials for High Performance Oxygen Reduction Reaction

JINXING 김지만*

성균관대학교 화학과

Polymer electrolyte membrane fuel cells (PEMFC) are appealing for transportation, stationary and portable applications due to their high conversion efficiency (up to 60%) and their zero pollutant and greenhouse gas emissions. Electrocatalytic oxygen reduction, the reaction at fuel cell cathodes, has been the focus of attention because of cathode catalyst layer used of expensive and less earth-abundant noble metals such as platinum and the oxygen reduction reaction (ORR) which typically occurs with overpotentials as high as 500-600 mV, which the higher than hydrogen oxidation reaction (HOR) on the anode side of fuel cells (over potentials as low as 50 mV). Since Jasinski's discovery that cobalt phthalovyanie exhibits catalytic activity for the ORR, research on metal-N4 macrocycles as a class of non-precious cathode catalysts has received considerable attention. Herein, we report the facile synthesis of Fe, N doped ordered mesoporous carbon (Fe-N-OMC) catalysts. The Fe-N-OMC catalyst secondary temperatures was found to display the best ORR activity with a highest onset potential of 1.003 V vs. real hydrogen electrode (RHE) and current density of 6.771 mA/cm^2, which was 29 mV and 0.888 mA/cm^2 even higher than that of the commercial 20 wt% Pt/C (Vulcan, loading: 1.02 mg$_{pt}$/cm^2) and highest half-wave potential of 0.851 V vs. RHE. Furthermore, durability and methanol tolerance tests showed that the catalyst had a better electrochemical stability than commercial Pt/C catalyst. X-ray photoelectron spectroscopy characterization of these catalysts was also conducted to identify the active nitrogen species for ORR.

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Self-Assembly Mechanism of Spiky Magnetoplasmonic Supraparticles

<u>주펑건</u> ZOUFENGMING[1] 이재범[2,*]

부산대학교 나노융합기술대학 [1]부산대학교 나노과학기술대학 [2]부산대학교 나노메디컬공학과

Concave nanoparticles (NPs) with complex angled and non-Platonic geometries have unique optical, magnetic, catalytic, and biological properties originating from the singularities of the electrical field in apexes and craters. Preparation of such particles with a uniform size/shape and a core-shell morphology represents a significant challenge, largely because of the poor knowledge of their formation mechanism. Here, we address this challenge and present a study of the mechanism of their formation for a case of complex spiky formed on different core particles that led us to conclusion that NPs with concave geometries can be, in fact, supraparticles (SPs) produced via self-assembly of smaller convex integrants. This mechanism is exemplified by the vivid case of spiky SPs formed via the attachment of small and faceted Au NPs on smooth Au-coated iron oxide (Fe3O4@Au) seeds. The diameter and surface roughness of the resulting spiky SPs is governed by the availability of the small faceted Au NPs. The theoretical calculations of energies of primary interactions ? electrostatic repulsion and van-der Waals repulsion elaborated for this complex case ? confirm experimental observation and self-limiting mechanism of SP formation. Weak stabilization of the constituent Au NPs participating in the self-assembly process results in the lattice-to-lattice connectivity and continuity of the metallic shell. Besides demonstrating the mechanistic aspects of synthesis of NP with complex geometries, this work also uncovered a facile approach for preparation of concave magnetoplasmonic particles. When combined with spiky geometry such bi-functional magnetoplasmonic SPs can serve as unique platform for optoelectronic devices and biomedical applications.

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Fluorescent and highly conductive iron-based nanocrystals via wet chemistry method

마오샹 권준영[1] 이재범[2,*]

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Iron based chalcogenides nanocrystrals (NCs) hold considerable promise for both solar energy conversion and electrical storage. Their utilization is hampered by lack of control over crystallinity and nanoscale organization of the homogeneous fabrications, the availability of high quality NCs of these materials will help us understand better both the photophysical processes in them and acquire building blocks to make better mesoscale materials from them. Therefore, two kinds of ~30nm diameter NCs FeSex (X=1, 2) have been synthesized and which display strong photoluminescence indicative of minimal defect density which are previously unavailable. FeSex (X=1, 2) displays photoluminescence (PL) peaks at 447nm and 462nm respectively while quantum yields are as high as 20%. Additionally, the synthetic route for iron based ternary chalcogenides NCs also have also been developed by doping Cr elements in the synthetic process, i.e., FeCr2Se4 and FeCr2S4 are synthesized through using a facile wet chemical method. FeCr2Se4 and FeCr2S4 NCs possessed narrow size distribution with high quality. FeCr2Se4 and FeCr2S4 NCs offer a promising conductivity for integration as electrical application. Importantly, these colloidal NCs can be considered be suitable for biomedical fluorescence marker and as the environmentally benign substitutes for optical, electronic and photovoltaic materials. Additionally, iron based bimetallic magnetic nanomaterials have been studied as the advancement.

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Protein Engineering for enhancing oxygen reduction reaction activity in noble gold nanoparticle arrays on peptide-SWNT superstructures

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There have been so many trials of understanding how to construct nanomaterial-protein superstructures and also a lot of successes have been built up. The stacked principles have been applied for designing the hybrid nanomaterial-protein superstructures can be binding inorganic or DNA or metal ions. Additionally, along with the advancement of the computer simulation, protein design has made great progress in the field of protein drug and related bioscience. Recently, our group designed the protein binding the surface of single wall carbon nanotube (SWNT) through the computation approach and also, they showed gold nanoparticles (gold NPs) directly assembled on the protein-SWNT nanocomposite. Here, we demonstrate that the gold NPs arrangements and sizes having ORR catalytic ability through manipulating the hybrid structure and multiple mutations with Cysteine residues in a designed protein bundle. It was observed that the size of gold NPs is 2 ? 3 nm and easily controlled by varying reduction time and precursor concentration. The position of gold NPs depends on the number of thiol group on Cys, and organized in outside of the nanocomposite by changing the number of a functional group that makes differs gold NPs density. The altering arrangement, size and density of gold NPs result in a significant change on ORR activity of the nanocomposites, and we confirmed the onset potential of the small and well-organized gold NPs arrangement is as high as the commercial Pt/C. This report suggests that the protein self-assembly structure has a potential to be a an easily modified, highly ordered electrocatalyst and further it is used in a marvelous electrode to other cell, for example, Li ion battery, Li air battery, and Fuel Cell.

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Striped C_{60} Pattern in a Cholesteric Liquid Crystal Medium

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A C_{60}-based Reactive molecule (C60RM) was newly synthesized and designed. Its chemical, thermal, structural and morphological properties were studied by the combined techniques of NMR and UV-Vis, DSC, TGA, X-ray diffraction, and POM. The striped C60RM patterns with regular clearance were successfully prepared via the one-dimensional (1D) pattern-forming state of an cholesteric liquid crystal (CLC) as a template. This work was supported by Converging Research Center Program (2013K000404), and BK21 PLUS Program, Korea.

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Self-assembly of peptides on primitive CVD graphene

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On primitive CVD graphene, we observed self-assembly of peptides designed to have π-π interaction with graphene with atomic force microscopy (AFM). Self-assembly of peptides on primitive graphene doesn't interfere with the π electron structure of primitive graphene. So functionalization of graphene surface by self-assembly of peptides can use unique properties of primitive graphene in efficient graphene application such as biosensor platform, ultrafast photodetector, or other bioelectronic devices. We designed β-sheet structure peptides by taking turns arranging hydrophobic (phenylalanine, F) and hydrophilic (lysine, K) amino acids and we observed it was self-assembled on large area successfully with protein pattern in AFM image. And we used chemical vapor deposition (CVD) graphene which don't have epoxide and hydroxyl group unlike graphene oxide (GO) or reduced graphene oxide (RGO). Also by using molecular dynamics (MD) simulations we expected how the peptides form β-sheet structure and assembled on graphene in solution.

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The preparation and properties of covalently cross-linked medium sulfonation degree SPEEK/Cs-MoPA/Ceria composite membranes for water electrolysis

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Covalently cross-linked medium sulfonation degree SPEEK/Cs-MoPA/CeO2 (sulfonated poly ether ether ketone) composite membrane was prepared for the polymer electrolyte membrane water electrolysis. Phosphomolybdic acid (MoPA) with a cesium was added to the SPEEK to increase proton conductivity. CeO2 was used to scavenge free radicals which attack the membrane in the water electrolysis and to improve the durability of the membrane. The composite membrane featured the electrochemical characteristics, such as 0.117 S/cm of proton conductivity at 80 ℃, 119.34% of water content and 64.85MPa of tensile strength.

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pH-responsive Spherical Nucleic Acid Cluster as a Platform for DNA Based Synergistic Anticancer Therapeutics

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포항공과대학교 화학과

We present herein a pH-responsive dynamic DNA nanomachine based on spherical nucleic acids (SNAs) assembly and evaluate the working inside the cell as a potential drug delivery carrier. Each SNA can be functionalized with various functional sequences, hence, we utilized the surface of the gold nanoparticles with bcl-2 antisense and i-motif binding sequences. Hybridization of i-motif sequence helped single SNAs clusterized in a size-controllable manner as drug loading cargo. Inside the cell, pH-responsive SNA cluster showed excellent drug release, forming single SNAs with respect to pH decrease at the late endosome. Furthermore, the expression of BCL-2 was down-regulated by single SNAs, leading a further apoptosis of the cancer cell by sensitizing the cancer cell simultaneously toward anticancer drug. Precisely programmed SNA based DNA nanomachine verifies the possibility of multifunctional therapeutic agents *in vitro*, and *in vivo* level.

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Scattering and near field induced enhanced photocatalytic activity of Au@TiO2 core-shell nanostructures

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이화여자대학교 화학나노과학과

Exploitation of solar energy to split water to generate hydrogen is an excellent tool to produce fuel without pollutants. The traditional titanium dioxide (TiO2) photocatalyst requires UV light to excite the electrons in the valence band, because of its wide band gap (e.g., 3.2 eV for anatase TiO2), which limits to use only about 4% of sunlight. Therefore, it has been a challenge to modify TiO2 that works under visible light, which covers 43% of solar spectrum. The conventional strategies to fabricate visible-light photocatalysts include doping, hybridization with other semiconductors, and dye-sensitization. Among these, inclusion of noble metals into TiO2 has drawn wide attention owing to their surface plasmon resonance (SPR) activity, which enables them to absorb visible light. Here, we developed gold (Au) spheres coated with TiO2 shell to study the role of scattering and near field enhancement (NFE) in elevating the electrons from the valence band of TiO2 to conduction band, and thereby improving the photocatalytic efficiency of TiO2. The evolution of hydrogen by water splitting was studied. We varied the size of Au NPs and thickness of TiO2 shell to obtain the optimum configuration showing maximum photocatalytic efficiency.

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DNA-templated silver nanoclusters as label-free, sensitive detection probes for potassium ion and nitric oxide

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포항공과대학교 화학과

DNA-templated silver nanoclusters (DNA-AgNCs) have highlighted as promising fluorescence material for sensing, bio-labelling, and bio-imaging. Herein, we developed two different types of DNA-AgNCs systems for the detection of potassium ion (K^+) and nitric oxide (NO) by utilizing structural change or transformation of template DNA. K^+ plays an important role in biological systems as it maintains extracellular osmolality, regulates concentration of other ions and balances the pH in living cells. In addition. NO has various biological functions such as cell proliferation, neurotransmission and antibacterial activity To detect In K^+ detection, thrombin binding aptamer was used as both template of AgNCs and binding probe of K^+. The fluorescence emission of DNA-AgNCs probe was diminished proportionally to the amount of K^+ detected, which transformed AgNCs-adapted structure into G-quadruplex. On the other hand, NO detection was accomplished using C12 sequence by NO-induced deamination of cytosine. Mutation of cytosine to deoxyuridine destabilized the DNA-AgNCs structure, resulting in quenching fluorescence intensity. The characteristics of these two highly quantitative detection probes were analyzed by UV absorption, fluorescence emission, and transmission electron microscopy (TEM) image. Each system provided detection limit of 6.2 μm for K^+ and 0.1 μm for NO. We expect that these system enable to open a new horizon for highly sensitive and selective detection systems.

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AuNP@PANI@Pt-transition metal Core-shell Nanostructure Electrocatalysts for Oxygen Reduction Reaction

이지은 김동하*

이화여자대학교 화학나노과학과

To design and fabricate highly active and durable oxygen reduction reaction (ORR) catalysts for the application in fuel cells (FCs) is mightily important. Also, the design of novel catalysts requires not only reducing the amount of Pt used but also enhancing catalytic activity and stability. Composites consisting of conducting polymers and metal nanoparticles are of great interest due to their combined properties of organic conductors and high surface area materials. Among conducting polymers, polyaniline (PANI) has been widely studied due to its unique thermal stability, high conductivity, environmental stability and reversible electrochemical and physical properties controlled by its oxidation and protonation. We suggest a unique strategy to generate core@shell nanoparticles based on Au NPs decorated with PANI shell. Concretely, Au NPs having PANI on the surface were first fabricated via atom transfer radical polymerization. Then, they were mixed with selected metal precursor solutions followed by reduction using reducing agent. The alloy metal NPs thus incorporated were distributed uniformly in the PANI polymer shells. We systematically investigate the structural alteration during the sequential synthetic process and compared the performance with respect to Pt-decorated AuNP@PANI structures.

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Fluorine-free blue phosphorescent emitters for efficient phosphorescent organic light emitting Diodes

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Two new Ir(III) compounds with sky-blue phosphorescence have been synthesized. These molecules have the general formula of Ir(C^N)2(L^X), where C^N = 2′,6′-dimethoxy-2,3′-bipyridine (OMe2pypy) and L^X = ancillary ligand such as acetylacetonate, acac (1), or 2-picolinate , pic, (2). Compounds 1and 2 emit bright blue phosphorescence with ?max = 462 -468 nm and quantum efficiencies of 0.49-0.54 in fluid and the solid state. Multi-layer electroluminescent devices using compounds 1and 2 as the dopant, MCPPO1(9-(3-(9H-carbazol-9-yl)phenyl)-9H-carbazol-3-yl)diphenylphosphine oxide) as the host and TSPO1 (diphenylphosphine oxide-4-(triphenylsilyl)phenyl) as the electron transport /hole blocking layer have been fabricated. These EL devices show blue color with high efficiency. The EL device of compound 2 at the doping level of 5 wt% shows the best performance with EQE of 12.1-15.3 % at the brightness of 10-1000 cd m-2 and the maximum current efficiency of 25.9 cd A-1.

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Synthesis and Characterization of Anthracene derivatives for Blue Organic Light-Emitting Material

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We have synthesized blue organic light-emitting diodes (OLEDs) material based on anthracene. Anthracene derivatives have been widely used as emitting materials in OLEDs because these derivatives have excellent photoluminescence. also, The advantages of anthracene are easy substitution and high thermal stability and high electronic stability. We expect in foreseeable future this moiety can using excellent blue OLED material. Thermal stability of anthracene derivatives was characterized by TGA and DSC and electronic stability was characterized by cyclovoltammetry.

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Graphitization of Nanodiamonds for Efficient Oxygen Reduction Reaction

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Graphitized nanodiamonds were prepared by the laser irradiation of colloidal solution using various solvents. The nanodiamonds were converted into a fully graphitized onion-like structure, which became a cage-like mesoporous structure by the degradation of graphitic layers. Alcohols, acetone, and acetonitrile are more efficient solvents for the graphitization compared to water and hydrocarbons. Therefore the number and morphology of the graphitic layers can be simply controlled by the solvent and laser-irradiation time. We suggest a graphitization model, in which the photocatalytic oxidation of the solvent accelerates the graphitization of nanodiamonds. The graphitized nanodiamonds were doped with the nitrogen and sulfur atoms in a controlled manner. In particular, the spherical graphitic layers were preferentially doped with the pyrrolic nitrogen that enhances remarkably electrocatalytic activity for the oxygen reduction reaction.

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Tin Germanium Sulfide Nanoparticles for Enhanced Performance Lithium Ion Batteries

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Composition-controlled ternary component chalcogenides germanium tin sulfide ($Sn_xGe_{1-x}S$) nanoparticles were synthesized by a novel gas-phase laser photolysis reaction of tetramethyl germanium, tetramethyl tin, and hydrogen sulfide mixture. Subsequent thermal annealing of as-grown amorphous nanoparticles produced the crystalline orthorhombic phase nanoparticles. All these composition-tuned nanoparticles showed excellent cycling performance of the lithium ion battery. The germanium sulfide nanoparticles exhibit a maximum capacity of 1020 mAh/g after 70 cycles. As the tin composition (x) increases, the capacity maintains better at the higher discharge/charge rate. This novel synthesis method of tin germanium sulfide nanoparticles is expected to contribute to expand their applications in high-performance energy conversion systems.

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Synthesis of QD-TiO_2 nanosheet hybrid nanostructures

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TiO_2 nanosheets (NS) of anatase, brookite structure were synthesized using hydrothermal method. Hybrid nanostructures were synthesized to combine synthesized TiO_2 NSs with CdSe/ZnS, InP/ZnS, $CH_3NH_3PbX_3$ Quantum Dots (QD).Also, Au nanoparticles were combined with QD-TiO_2 hybrid nanostructures. The morpholgy and structure of the products were analyzed by scanning electron microscopy (SEM), energy dispersive X-ray spectroscopy (EDX), transmission electron microscopy (TEM) and X-ray diffraction (XRD).We observed that as-synthesized hybrid nanostructures has improved efficiency for photocatalysis through water splitting and methylene blue splitting experiment.

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Synthesis of Transition metal doped Ta_2O_5, TaON, Ta_3N_5 Nanocrystals

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Photoreductions of CO2 under visible light irradiation have been increasingly receiving considerable interest not only from environmental and long term energy-security view points but also as a crucial scientific issue in the field of artificial photosynthesis. Herein we synthesized the Ta₂ O?, TaON and Ta₃ N? nanocrystals as photocatalysts using a sol-gel method. The transition metal were doped with a concentration of 1~10 atomic %. We examined the photocatalytic activity of the doped nanocrystals in a comparison with undoped nanocrystals, We also investigated the electrocatalysts for the oxygen evolution and reduction reactions.

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Tin Nanocrystals in Lithium Ion Batteries and thier Phase Evolution

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We comparatively investigated how the phases of Sn, tin sulfide (SnS), and tin oxide (SnO_2) nanocrystals (NCs) changed during repeated lithiation/delithiation processes. All NCs were synthesized by a convenient gas-phase photolysis of tetramethyl tin. They showed excellent cycling performance with reversible capacities of 700 mAh/g for Sn, 880 mAh/g for SnS, and 540 mAh/g for SnO_2 after 70 cycles. Tetragonal-phase Sn (β-Sn) was produced upon lithiation of SnS and SnO_2 NCs. Remarkably, a cubic phase of diamond-type Sn (R-Sn) coexisting with β-Sn was produced by lithiation for all NCs. As the cycle number increased, R-Sn became the dominant phase. First-principles calculations of the Li intercalation energy of R-Sn (Sn_8) and β-Sn (Sn_4) indicate that Sn_4Li_x ($x \leq 3$) is thermodynamically more stable than Sn_8Li_x ($x \leq 6$) when both have the same composition. R-Sn maintains its crystalline form, while β-Sn becomes amorphous upon lithiation. Based on these results, we suggest that once R-Sn is produced, it can retain its crystallinity over the repeated cycles, contributing to the excellent cycling performance.

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Phase Evolution of $(GeTe)_mBi_2Te_3$ ($m \geq 3$) Nanowires and Their Electrical Conductivity

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Phase change nanowire (NW) has emerged as critical materials for fast switching-speed non-volatile memory devices. As one of promising candidate, $(GeTe)_mBi_2Te_3$ (GBT) nanowires (NWs) were synthesized with wide range composition tuning, $m \geq 3$, by a chemical vapor transport method. The NWs exhibit composition-dependent phase evolution from the cubic to hexagonal phase, with the superlattice structures with periodic slabs of 2.2~3.8 nm, corresponding to m = 3~8. They were grown along the $[111]_C$ ($=[0001]_H$ or c-axis) or [011] direction. *In situ* temperature-dependent transmission electron microscopy revealed that the stability of the hexagonal phase increases with m. First-principles calculations of $(GeTe)_mBi_2Te_3$ and $(GeTe)_mSb_2Te_3$ ($m \leq 8$) series was performed for the hexagonal and cubic phase superlattice structures. The structure and the phase evolution were explained using the increased thermodynamic stability of the hexagonal phase relative to the cubic phase with decreasing m. Measurement of the current-voltage curve for individual NW showed that the resistivity of the [111] direction is higher than that of the [110] direction, which was also supported by the calculations.

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$(GaP)_{1-x}(ZnS)_x$ Alloy Nanowires

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Semiconductors with direct band gaps corresponding to the energy of visible light have many important applications such as light emitting diodes and photocatalysts. The $(GaP)_{1-x}(ZnS)_x$ quaternary alloy nanowires were synthesized with a full-range composition tuning, via catalyst-assisted chemical vapor transport method. The morphology, composition, and crystal structure of the as-synthesized nanowires were investigated by scanning electron microscopy, energy dispersive X-ray spectroscopy, high-resolution transmission electron microscopy (HRTEM), and X-ray diffraction pattern. As the x (ZnS composition) increases, the phase of nanowires evolved continuously from the zinc blende GaP to wurtzite ZnS, through coexisting of two phases at $0.3 < x < 0.7$. We measured the UV-visible spectrum and laser photoluminescence as a function of composition. Remarkably, the band gap increases non-linearly with the composition, from 2.2 eV to 3.5 eV. We also observed the power-dependent blue shift of the photoluminescence. The decay time of photoluminescence has been monitored as a function of laser power and composition. The photodetectors that consisted of single nanowire has been fabricated to show an excellent response sensitivity.

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Synthesis of Anthracene Derivative for Organic Light-Emitting Diodes

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경상대학교 화학과 [1]경상대학교 나노신소재공학부

We have synthesized asymmetrical blue organic light-emitting diodes (OLEDs) material basedon anthracene. Anthracene derivatives have been widely used as emitting materials in OLEDsbecause these derivatives have excellent photoluminescence. Anthracene derivatives have beenextensively studied and developed as light-emitting materials in OLEDs owing to their interesting electroluminescence (EL) properties. In principle, the asymmetric structure can control the electronic properties due to different dipoles and can also inhibit intermolecular interaction dueto reduced stacking, compared with a symmetric structure. Also, The advantages of anthraceneare easy substitution at the 9 and 10 positions, high thermal stability and high electronic stability. We expect in foreseeable future this moiety can using excellent blue OLED material.

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Enhanced light extraction of GaN-based blue light emitting-diodes with photonic crystal patterned sapphire substrate

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In order to enhance light extraction efficiency from GaN-based blue light emitting-diodes (LEDs), we fabricated a two-dimensional (2D) air-hole photonic crystal (PC) array on the sapphire substrates. The 2D air-hole PC array was fabricated by a combination of polystyrene (PS)-based nanosphere lithography (NSL) and inductively-coupled-plasma (ICP) etching process. Using the NSL, the SiO_2 air-hole PC array were fabricated on the sapphire substrate in order to be used as etching mask for transferring to the underlying sapphire substrate. From the ICP etching process using BCl_3 and Ar gas mixture, subsequent pattern transfer into the sapphire substrate was performed. Then, GaN epilayer was grown on top of the 2D PC patterned substrate by metal-organic chemical vapor deposition (MOCVD) and conventional LED structure was subsequently fabricated. The structural and morphological properties of the patterned sapphire substrate and the full processed GaN-based LED were investigated by scanning electron microscope (SEM). The current-voltage (I-V) characteristics and optical properties of the full processed LED were measure by probe station system and spectrophotometer.

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The realization of field-induced photoluminescence switching display using quasi-type II CdSe/CdS quantum rods

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We introduce the field-induced photolumincescence (PL) switching display using quasi-type II CdSe/CdS quantum rods (QRs). We synthesize quasi-type II red-colored, rod-shaped CdSe/CdS QRs by seed-growth two-step method using different reactivity between octadecylphosphonic acid (ODPA) and hexylphosphonic acid (HPA). In case of quasi-type II CdSe/CdS QRs, the electrons delocalized throughout the core and shell and the holes confined in the core due to its band alignment. For this reason, the quasi-type II CdSe/CdS QRs can be aligned by the electrophoretic force and can allow field-induced PL switching. We aligned the QRs by applying the voltage with sin wave and we turned off the aligned QRs by applying the voltage with square wave. The contrast ratio controlled by changing the applied voltage.

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Polarized, white phosphor converted LEDs using remote phosphor layer sandwiched between reflective polarizers and short wavelength pass dichroic filters

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In this study, an efficient polarized, white phosphor converted, light-emitting diode (pc-LED) using a remote phosphor layer sandwiched between a reflective polarizer film (RPF) and a short wavelength pass dichroic filter (SPDF), which transmit blue wavelength regions and reflect yellow wavelength regions, is introduced. Yellow phosphor layer is fabricated using $Y_3Al_5O_{12}$:Ce^{3+} (YAG) yellow phosphor purchased from a phosphor company (Merck Co. Ltd.). We compare four different types of remote phosphor layers: conventional, RPF-capped, SPDF-inserted and RPF/SPDF-sandwiched remote phosphor layers over a blue LED. The SPDF is located backside of RPF. The on-axis luminous efficacy of the the unpolarized, SPDF-inserted phosphor layer is 1.40 times higher than that of the unpolarized, conventional remote phosphor layer. The on-axis luminous efficacy of the RPF/SPDF sandwiched phosphor layer is 1.90 times higher than that of the RPF-capped phosphor layer. The on-axis luminous efficacy of the the unpolarized, conventional remote phosphor layer is 1.39 times higher than that of the RPF/SPDF sandwiched phosphor layer. The polarized white light demonstrated in this work has increased potential for a wide range of traditional lighting applications, including LCD backlighting, outdoor lighting, indoor lighting, and automobile lighting.

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Correlated color temperature tunable white-light-emitting diodes using quantum dot coated short-wavelength pass dichroic filter

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In this study, we design the remote-type white-light-emitting diodes (W-LEDs) combined with $AgIn_5S_8$-ZnS (AIS-ZS) alloyed quantum dots (QDs) and four different types of short-wavelength pass dichroic filter (SPDF), which transmit blue region and reflect green to red region, in order to tune correlated color temperatures (CCTs, K) and color rendering index (CRI, Ra). The AIS-ZS QDs are synthesized by using colloidal hot injection method and the quantum yield (Q.Y.) of the QDs is about 65%. To make QD films on SPDFs, the QDs were mixed with poly(methyl methacrylate) (PMMA) in toluene and dimethylformamide (DMF) solution and spin coated. We use the four different types of SPDFs with changing the range of reflecting wavelength from greenish to reddish region. We changed the thickness of QDs film on SPDFs by increasing the number of layers and changed the reflecting wavelength to reddish region of QDs film coated SPDFs to tune the CCTs and CRI from cool white to warm white. The optical properties of QDs were characterized by UV-Vis spectroscopy, photoluminescence (PL) and electroluminescence (EL).

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Synthesis and Electroluminescence Properties of Highly Efficient Dual Core Chromophores for Blue Emission

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Highly efficient blue emitting materials consisting of dual core derivatives with phenyl and/or naphthyl side groups and asymmetric or symmetric structures were designed and synthesized. The asymmetric structures 1-naphthalen-1-yl-6-(10-phenyl-anthracen-9-yl)-pyrene (Ph-AP-Na) and 1-(10-naphthalen-1-yl-anthracen-9-yl)-6-phenyl-pyrene (Na-AP-Ph), and the symmetric structures 1-phenyl-6-(10-phenyl-anthracen-9-yl)-pyrene (Ph-AP-Ph) and 1-naphthalen-1-yl-6-(10-naphthalen-1-yl-anthracen-9-yl)-pyrene (Na-AP-Na) were synthesized. Of the synthesized compounds, Na-AP-Na was found to exhibit the highest EL device efficiency of 5.46 cd A-1. Ph-AP-Na, Na-AP-Ph, Ph-AP-Ph, and Na-AP-Na exhibit EL maximum values of real blue color in the range 455 nm to 463 nm. The y values of their color coordinates are within the range 0.125 to 0.142, so these compounds exhibit good blue color coordinates for displays. The lifetime of Na-AP-Na device showed more than three times longer than AP dual core (1-anthracen-9-yl-pyrene) device.

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Haze control of Ag nanowire-based transparent conductive films

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Ag nanowire-based transparent conductive films (TCF) has become one of the strong candidate which can replace Indium-tin-oxide (ITO) TCF. However, the optical properties, especially the haziness of a TCF remain a problem yet. The haziness is originated from the random reflections from the silver nanowire surfaces. To reduce such reflections, people have tried many different studies including the control of Ag nanowire dimensions, thinner and longer wires, and hybridization with other conducting materials such as carbon nanotubes (CNT), graphene, and conducting polymers. All these approaches are to reduce the Ag coverage on a surface to minimize the random reflections. Although these approaches showed reduced haziness in the TCF, the intrinsic haziness of the TCF still remain a problem especially when the sheet resistance become smaller, due to the increasing amount of Ag nanowires.In our approach, we attempt to control the haziness of a Ag nanowire-based TCF using optical overcoating layers. High refractive index overcoating layer can effectively reflects back the randomly reflected light to the film layer so that haziness of a TCF film can be reduced from 1.2% to as low as 0.9% (including PET film haziness). We have prepared several overcoating layers with different refractive index value and compared the haze changes. Furthermore, these overcoating layers can enhance the mechanical strenght of TCF for the following patterning processes.

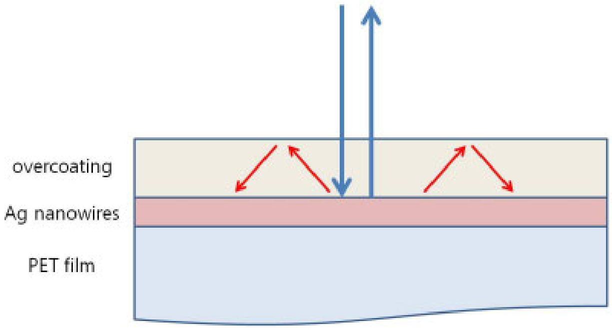
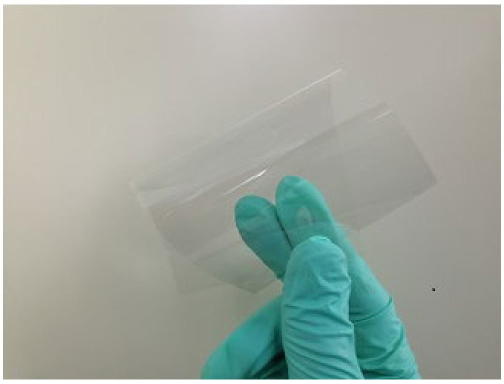


그림 1. random reflection in the high refractive index overcoating layer on Ag nanowire TCF



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Synthesis and Electroluminescence Property of New Hexaphenyl Benzene Derivatives Including Amine Group for OLED

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Five new Blue emitting compounds for OLED based on hexaphenyl benzene moiety. Physical properties by the change of the substitution groups of the synthesized materials were systematically examined. Photoluminescence(PL) spectrum of the synthesized materials showed maximum emitting wavelengths of about 400~447 nm in solution state and 451~461 nm in film state, indicating deep blue emission color. OLED devices were fabricated by the synthesized compounds using vacuum deposit process as a emitting layer. Device structure was ITO/2-TNATA 60nm/ NPB 15nm/ EML 35nm/ TPBi 20nm/ LiF 1nm/ Al 200nm.

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A facile synthesis of chetnut-bur-like palladium nanostructures for enhanced electrocatalytic activity

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In this work, we demonstrate a fast and facile one-pot synthesis method of chestnut-bur-like palladium nanostructures with highly open structure and huge surface area in aqueous solution by using Na2PdCl4, cetylpyridinium chloride (CPC) and L-ascorbic acid (AA) as a precursor, surfactant and reducing agent, respectively. The synthesized chestnut-bur-like palladium nanostructures had an average overall size of 70 nm and were composed of needle-like arms with 2.3 nm average thickness. Time evolution of Pd nanostructures implied that small Pd particles generated at the early stage of the reaction by fast reduction grew via particle attachment growth mechanism. Moreover, the morphology of Pd nanostructures could be controlled by changing the concentration of CPC aqueous solution; depending on the amount of CPC, the reduction rates varied the morphology of the Pd nanostructures. Electrocatalytic activities toward ethanol oxidation reaction were measured compared to Pd cube, Pd octahedron and commercial Pd/C. Because of their huge electrochemically active surface area and high density of catalytically active sites, chestnut-bur-like Pd nanostructures showed greater electrocatalytic activity toward ethanol oxidation than other three Pd nanocatalysts.

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Selective and effective doping of semimetal antimony at the edge of graphene nanoplatelets via mechano-chemical reaction and its electrochemical properties

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It is an epoch-making work to show the doping of semimetal antimony (Sb) at the edge of graphene nanoplatelets through simple mechano-chemical reaction and effective electrocatalysts for cathodic oxygen reduction reaction (ORR). We have fabricated facilely and in quantity antimony doped graphene nanoplatelets (SbGnP) by ball milling of the pristine graphite with antimony. It confirmed the doping of antimony at the edge of graphene nanoplatelets with various analysis technologies and SbGnP contained a lot of antimony about 1.18 at%. Additionally, it found that the enough energy generate from the broken carbon-carbon bond to be even reactive with semimetal, antimony, or to fix directly antimony at the edge of graphite. As a result, SbGnP was a more active and durable catalyst for oxygen reduction reaction (ORR) in alkaline condition than the pristine graphite or commercial Pt/C electrocatalyst.

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The effect of electron beam irradiation on Ni/graphene hybrids

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Graphene-based materials are good for energy storage applications because graphene has a broad electrochemical range, a chemical stability, a high electric conductivity and a large specific surface area. At first, to fabricate energy storage materials with flexible delaminated structure, graphene oxide was hybridized with nickel particles. And then, morphology of prepared hybrid materials was changed by simple and facile synthetic method using electron beam irradiation. According to X-ray diffraction and X-ray absorption spectroscopic analysis, nickel nanoparticles were homogeneously distributed on graphene nanosheets. Also, TEM images of these hybrids show different mophology and several defects developed by electron beam irradiation. The Ni/graphene hybrids exhibit higher energy storage properties than those of graphene nanosheets and nickel nanoparticles. And the new synthetic method can be used to improve electrochemical properties without any deterioration of the fundamental crystal structures.

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LED용 형광체의 온도에 따른 형광 특성 측정 장치 개발 및 응용

권은실 노경원[1,*]

(주)신코 연구개발부 [1](주)신코 중앙연구소

최근, LED 중 친환경적이며, 긴 수명을 가지고 있으므로 형광등을 대체할 수 있을 것이라 기대 하고 있는 백색 LED 에 관한 연구가 관심을 모으고 있다. 백색 LED 는 발광 다이오드를 기반으로 LED 로부터 나오는 빛을 적, 황, 녹청색 광인 가시광선으로 전환하는 형광체를 이용하여 태양광의 광 분포와 유사한 백색광을 방사 할 수 있게 된다. 본 연구에서는, 형광 분광 분석 장비에 손쉽게 장착 할 수 있고, 열전 소자를 이용하여 형광체 시료의 온도를 상승 및 냉각 시킬 수 있는 Peltier powder cell holder 를 새로이 개발하여 형광체의 온도에 따른 형광 특성을 조사하였다. Peltier powder cell holder 는 시료의 온도는 0℃ ~100℃까지 변화 시킬 수 있으며 최대 온도 상승 속도는 30℃/min 이다. 본 장치를 이용하여 측정한 결과, 황색, 적색, 녹색 LED 형광체는 온도가 증가 할수록 형광 세기가 감소하는 경향을 보였으며, 그 변화율은 약 11%/℃ 정도였다. 또한, 온도 상승에 따라 최대 발광 파장이 장파장으로 조금씩 이동하는 경향을 보임을 확인 할 수 있었다.

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다양한 환원제와 반응조건을 이용한 여러 형태의 금속나노입자 제조

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금속 나노입자는 입자의 크기 및 형태에 따라 입자 표면의 국부 플라즈몬 공명현상(Localized Surface Plasmon Resonance, LSPR)에 의해 광학적 특성이 달라진다. 이와 같은 특성은 나노입자의 크기와 모양에 영향을 받으며, 이에 대한 특성 파악과 응용분야를 찾기 위한 연구가 세계적으로 활발하게 진행되고 있다. 이러한 연구의 일환으로, 본 연구에서 금속이온(Au,Ag,Pt)을 Trisodium citrate 와 sodium borohydride 환원제를 이용하여 환원시키면 환원된 금속 원자들이 서로 모여 금속 나노 입자를 형성하는 방법을 이용하여 실험하였다. 제작 조건으로 화학적 환원법, 씨드(seed)를 이용하는 방법, 광화학적 환원법 등을 이용하여 크기와 모양이 조절된 나노물질을 제조하였다. 합성된 금속 나노 입자는 UV-Vis absorption spectroscopy 과 transmission electron microscopy(TEM)을 이용하여 확인하였다.

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Blue Emitting Antracene Derivative for OLED

마재열 김란 김형남 천예림 전찬우[1] 김윤희[*] 권순기[2,*]

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Organic light emitting devices (OLEDs) have been attracting considerable attention for potential application in flat-panel displays. Efficient blue-light OLEDs are of particular interest, because they are desired for use as blue light sources in full color display applications. Significant progress in materials synthesis and device construction has led to the realization of full color as well as white OLEDs with improved efficiencies and lifetimes. Extensive efforts have been made to develop high performance materials with desirable properties, and devices with optimized architectures to develop marketable OLEDs.

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Preparation of Reduced Graphene Oxide/Co(OH)$_2$ Nanosheet Composite as Electrocatalyst for Oxygen Reduction Reaction

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가톨릭대학교 화학 [1]가톨릭대학교 화학과

Nanosheets of cobalt hydroxide have been successfully coated on reduced graphene oxides via electrostatic self-assembly. The cobalt hydroxide nanosheet was prepared by the exfoliation of layered alpha cobalt hydroxide nanocrystals, in which the green color of the alpha cobalt hydroxides was gradually changed into pink. This visible transition occurred due to the structural change of alpha cobalt hydroxide into individual beta cobalt hydroxide nanosheets. Mixing of two colloidal suspensions, the exfoliated beta hydroxide nanosheets and the graphene oxides, dramatically produced a well-oriented two-dimensional hybrid material with a maximum face-to-face contact. High-resolution TEM measurements revealed that the thermal decomposition of the hybrid nanosheets yielded homogeneous Co_3O_4 nanoparticles with a narrow size range of 5 nm on the reduced graphene oxide layers. The strongly coupled hybrid nanosheets of Co_3O_4/reduced graphene oxide have been used as an electrochemical catalyst for oxygen reduction reaction in alkaline electrolyte.

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Tunable Decoration of Gold Nanoparticles on Mg_2Al Layered Double Hydroxide Nanosheet for Reusable Catalysts

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Uniform 2-dimensional hybrid catalyst consisted of gold nanoparticles decorated on layered double hydroxide (LDH) nanosheet has been prepared by the in-situ chemical reduction of gold chloride in the colloidal suspension of LDH nanosheet. The LDH nanosheets with a high-level of positive charge density were produced by the exfoliation of LDH crystals into single hydroxide layers, which leads to electrostatic interactions between the LDH layers and gold precursors and/or gold nanoparticles. The gold nanoparticles were homogeneously synthesized on the LDH nanosheet with a uniform size around 20 nm. In the absence of the LDH nanosheet, the gold nanoparticles were readily precipitated due to a fast aggregation into large particles. This 2-dimensional hybrid material showed a high stability in water and exhibited an excellent catalytic activity and durability for the reduction of 4-nitrophenol into 4-aminophenol in the presence of $NaBH_4$. The utilization of the double hydroxide nanosheet as a new type of supports for transition metal NPs will dramatically improve the durability in heterogeneous catalysis.

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Synthesis of a pseudocapacitor electrode with polyaniline and hollow structure WO3 in nickel foam

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성균관대학교 화학과

Supercapacitor or electrochemical capacitor has received great research because its properties of high power density, long cycle life and fast charging / discharging rate. Depend on the charge store mechanism, supercapacitor contains electrical double layer capacitor and pseudocapactor, and the latter has attracted more attention due to its fast and reversible faradic charge storage capability. Here we chose hollow material due to their high purity, large surface area and homogeneous morphology. Hollow structure PbWO4 was as the original material to make dendrite and sphere WO3. Later adulterate the hollow WO3 into aniline solution to make WO3/polyaniline copolymer. Kirkendall effect was used to explain the formation mechanism of the hollow WO3 shells.This work was supported by the Energy & Resource of the Korea Institute of Energy Technology Evaluation and Planning(KETEP) grant funded by the Korea government Ministry of Trade Industry and Energy (No.2010501010002B)

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Layered Sodium Cobalt Oxides/Graphene Oxide Nanocomposites for Improvement of Capacity Retention in Sodium Ion Batteries

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Na_xCoO_2 has been studied as a cathode material in sodium ion batteries. It has been reported that Na_xCoO_2has four different crystal phases. In each phase, the Co ions occupy the octahedral sites and CoO_6octahedra are connected by edge-sharing. The Na^+ ions can occupy the octahedral and prismatic sites, which are sandwiched by CoO_2 slabs. According to the stacking sequence of the oxygen layers, the two-layer structure of repeated CoO_2 slabs has γ phase in $0.6 \le x \le 0.75$ and the three-layer structure of repeated CoO_2 slabs can have β phase in $0.55 \le x \le 0.6$, α phase in $1 \le x \le 0.9$, and α' phase at x=0.75. In this study, stoichiometric $NaCoO_2$ (NCO) was anchored on graphene oxide (GO) and used as a cathode material for the improvement of cycle stability in sodium Ion batteries. Co_3O_4 was first prepared on GO and then converted to NCO by heat-treating with Na_2O_2 in an inert atmosphere at 550℃ (to minimize the loss of GO). During this process, GO was simultaneously reduced to graphene to provide NCO with a conducting network and possibly structural stability (NCO/GO). The former is important because the stoichiometric NCO with O3-type layered structure is in an electronically semiconducting state, in contrast to non-stoichiometric NCO (metallic). Therefore, the excellent electrochemical properties in NCO/GO could be expected due to nanoparticles anchored on graphene. As expected, the composite showed the improved capacity retention, which was substantially better than the pristine NCO. Moreover, a capacity of NCO was higher the pristine NCO. Multi-step phase transition was not altered, but the capacity fading was negligible during 50 cycles. We are currently comparing the electrochemical performance of NCO/GO, which was synthesized with a slight excess of Na_2O_2 (1.1 eqv.), with pristine NCO.

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Improvement of initial coulombic efficiency of Li-ion battery using mesoporous manganese-nickel oxides electrode

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Owing to the rapid development of portable electronic devices, there is an increasing demand for Li-ion batteries with high energy density, long cycle life and initial coulombic efficiency.Graphite-based materials are generally used as anode materials in commercial LIBs. However, as anode material for LIBs, graphite is limited by its low theoretical specific capacity of 372 mAhg?1 and limited rate capability. Transition metal oxides with higher energy density (such as MnOx, NiO, SnO2, Co3O4, WO3) have drawn much attention as the desired candidates for anode materials to satisfy the higher energy storage requirements. Among these transition metal oxides, manganese oxide is of great importance as anode materials for LIBs due to its low operating voltage, low toxicity, low cost, and widespread availability. However its irreversible capacity comes to about 40% of initial capacity, the initial coulombic efficiency needs improvement in order to commercialize meso-Mn2O3 as the anode material of LIBs. Therefore, meso-NiMnO3 was selected to decrease the initial irreversible capacity. In this study, Meso-NiMnO3 was synthesized using KIT-6 as template and characterized using XRD, Nitrogen sorption technique and SEM(scanning electron microscopy),electrochemical techniques

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Site-Selective Growth of Palladium on Au Triangular Nanoplate

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성균관대학교 화학과

We investigated the site-selective reduction of Pd ions on three different sites of Au triangular nanoplate namely; vertex, edge and terrace. Vertex site has the highest surface energy than the others resulting to more unstable state. Ag layer was deposited on the Au triangular nanoplate by using the ascorbic acid, followed by galvanic replacement reaction between the Ag layer and Pd precursor. We found that there are two important factors for the site-selective growth of Pd on the Au triangular nanoplate. Firstly, we tuned the concentration of Hexadecyltrimethyl-ammonium bromide (CTAB) which is served as capping agent. CTAB molecules block specific facets based on the concentration. Therefore, Pd ions were selectively reduced on the vertex and edge site of the Au triangular nanoplate. Secondly, growth direction of Pd can be controlled by the presence or absence of iodide ions. Iodide ions usually favor to adsorb on the Au(111) facet resulting in the reduction of Pd ions on the terrace of Au triangular nanoplate. Depending on the concentration of CTAB and the existence of iodide ions, we obtained Au-Pd nanoplates with four representative morphologies. The names of the synthesized four structures are apex-preferential, rim-preferential, bulky-granule and tiny-granule. Moreover we suggest a mechanism to understand this phenomenon. Lastly, we characterized four structures by using scanning electron microscopy (SEM), transmission electron microscopy (TEM), UV-vis-near IR spectroscopy and X-ray diffraction (XRD) patterns.

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Tuning the Surface of Au-Ni-Au Multiblock Nanorods selectively treated with N719 Dye: Toward Reversible On/Off Switching of Surface Plasmon Resonance

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We synthesized Au-Ni-Au multi-block nanorods (NRs) using anodized aluminium oxide (AAO) templates by electrochemical deposition method and observed surface plasmon resonance (SPR) coupling after selectively attaching N719 dye molecules on the Ni segment. Typically, it is difficult to observe the SPR phenomenon of Ni nanomaterials in UV-vis spectra because the Ni nanomaterals have relatively optical inactive characteristics. However we can observe SPR coupling in Au-Ni-Au multi-segmented NRs since electron oscillation of Au causes free electron oscillation of Ni. In this report, we observed that longitudinal mode of Au-Ni-Au NRs disappeared in the case of N719 attached to Ni site. Then, we confirmed that SPR coupling reappeared after detaching N719 dye molecule. Therefore, it is proved that we could control the reversible SPR coupling by tuning the surface of Au-Ni-Au NRs. The retained junctions between multi-blocks confirmed by SEM images do not affect the SPR coupling. Selectively treated with N719 dye on the surface of Ni was confirmed by Raman spectroscopy and mapping image system.

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Graphene nanomesh for enhanced Raman signal

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In this work, we fabricated graphene nanomesh (GNM) using Pt nano-network as a pattern mask and showed its potential as a SERS substrate. GNM exhibited much higher Raman signal than that of pristine graphene since GNM has a large amount of edge that acts as chemically hot spots. We further controlled the neck width, the smallest distance between pores, to correlate electronic properties and Raman enhancement. As decreasing the neck width, the Fermi level of GNM shifts, resulting in the enhancement of charge transfer. Characterization was done by Scanning Electron Microscopy and Raman spectroscopy.

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Morphology Evolution and Surface Plasmon Observance of Gold Nanorod-in-a-Multi-Nanoshell by Galvanic Replacement

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Gold nanorod-in-a-multi-nanoshell nanoparticles have been prepared by repeated silver coating and subsequent galvanic replacement. As the number of shell increases, a clear morphology transformation was observed under scanning electron microscopy (SEM) showing that the anisotropic gold nanorod gradually changes to an isotropic nanoparticle. Results from transmission electron microscopy (TEM) showed that the multiple-nanoshell around the gold nanorod was indeed obtained. Optical spectra of the well-dispersed colloidal nanoparticle solutions having different number of shells were investigated by using UV-vis spectrophotometry and showed that the transverse and longitudinal dipole mode merged into a single dipole mode which further confirms the shape transformation. We found that at 100 nm size regime, the gold nanorod-in-a-multi-nanoshell nanoparticles suppressed the quadrupole surface plasmon mode as opposed with comparable size of solid and hollow nanoparticles. Similar trend was observed whether the aspect ratio (length/width) of the core gold nanorod was changed or the distance and thickness of the shell were precisely controlled in the range between 5 to 1 nm.

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Dielectric properties of tungsten-bronzes β- and β'-$SrTa_2O_6$

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Strontium ditantalum oxide $SrTa_2O_6$ shows a polymorphism including tungsten-bronze type β- and β′-phases. These two forms of $SrTa_2O_6$ have similar lattice structures, but the latter (tetragonal) has the higher crystal symmetry and the larger cell volume than the former (orthorhombic). While the dielectric behavior of $SrTa_2O_6$ has been studied for a while, no attention was paid to the structure-property relationship in the past. In this regard, we measured the dielectric constant κ of β- and β′-$SrTa_2O_6$ in the range 12-400 K, using an LCR meter. Over the entire temperature range in this study, κ(β′-$SrTa_2O_6$) was a little higher than κ(β-$SrTa_2O_6$), and both β′- and β-$SrTa_2O_6$ exhibited a broad peak of κ around 70 K. For understanding the observed dielectric characteristics, we focus on the local geometry of TaO_6 of each phase.

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Experimental (SERS) and Theoretical (FDTD) studies on Au Nanparticles/Mesoporous Platinum Thin Films

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We reported the study about the experimental and theoretical SERS effect on Au nanoparticles / mesoporous Platinum thin films. In order to find suitable SERS substrate, we synthesized gold nanoparticles with different size from 13 nm to 80 nm to be adsorbed on mesoporous Pt films. Using 4-aminobenzenethiol (4-ABT) as probe molecules, the substrate of gold NPs on mesoporous Pt thin films showed strong SERS signals than of gold NPs on Silicon wafer due to the interactions of interlayer between gold nanoparticles and mesoporous Pt thin films. So-called 'hot spot' in an interlayer of Au NPs and mesoporous Pt thin films makes strong local electric fields and it can lead SERS effect. This SERS effect of the interlayer of Au NPs and mesoporous Pt films was confirmed on the computational results, which were applied by the finite difference time domain (FDTD). Furthermore, high electric field enhancement was shown at the substrate of 50 nm Au NPs on mesoporous Pt thin films. This is consistent with the experimental results. Based on experimental and theoretical results, we demonstrate that the electric field enhancement in the junction region of Au NPs and mesoporous Pt films leads SERS effect.

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Surface?Engineered Nanomaterials as X?ray Absorbing Adjuvant Agents for Auger?Mediated Chemo?Radiation

이상민

가톨릭대학교 화학과

We demonstrate a prototype approach to formulating gold nanoparticle (AuNP)-based X-ray absorbing adjuvant agents through surface-engineering of cisplatin pharmacophore (Pt) with lipoic acid-modified polyacrylate (Pt-AuNPs). Design of Pt-AuNPs was examined and further validated using a combination of physicochemical characterization methods. Our results show Pt-AuNPs exhibits very high capacity for Pt-loading via the mechanism of multidentate coordination between Pt(II) ions and surface-bound polyacrylate. The Pt-AuNP vector demonstrated excellent colloidal stability in an acid-sensitive manner that enables Pt drug-release, and exhibited high in vitro cytotoxicity to the cancer cell lines MCF-7 and SK-OV-3. Secondary electron emissions from both Pt(II) and AuNPs are triggered by an external ionizing radiation source via the Auger cascade. As a result, Pt-AuNPs exhibit therapeutic potential as an adjuvant agent for concurrent chemo-radiation cancer therapy.

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Carbazole and Carboline-based Host Materials for High Efficiency Blue Phosphorescent Organic Light-Emitting Diode

김형종 신지철 엄현아 조민주 권장혁[1] 최동훈[*]

고려대학교 화학과 [1]경희대학교 정보디스플레이학과

Phosphorescent organic light-emitting diodes (Ph-OLEDs) have been developed because of high quantum efficiency of phosphorescent emitting materials. Some specific organic charge transport and emitting materials have been employed in blue Ph-OLEDs. However, the most critical materials for improving the device performances are host materials in emitting layer. The host materials with high triplet energy manage hole and electron balance in the emitting layer and determine the high quantum efficiency of Ph-OLEDs. In this study, 9-(6-(9H-Carbazol-9-yl)pyridin-3-yl)-6-(9H-carbazol-9-yl)-9H-pyrido-[2,3-b]indole (pPCB2CZ) and 9-(6-(9H-Carbazol-9-yl)pyridin-2-yl)-6-(9H-carbazol-9-yl)-9H-pyrido-[2,3-b]indole (mPCB2CZ) were synthesized as bipolar high triplet energy host materials for blue Ph-OLEDs. Compared with carbazole, α-carboline and pyridine subunit makes electron abundant and can improve electron transport properties. These bipolar host materials were highly effective to yield a high efficiency blue Ph-OLED using FIrpic as a blue dopant. High external quantum efficiencies of 27.1% ~ 28.3 % were demonstrated in p-n-p junction blue Ph-OLEDs.

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Phase formation of transition metal sulfide nanoparticles by the annealing atmosphere

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성균관대학교 화학과

Surfactant-free synthesis of the Cu_2ZnSnS_4(CZTS) and the $CuInS_2$(CIS) were prepared using facile sonochemical process under ambient conditions. CZTS nanoparticles were synthesized with metal chlorides and sulfur powder in oleylamine. CZTS nanoparticles were dispersed in hexanol for prepared colloidal solution and deposited by Mo substrtae using electrophoretic deposition. As-deposited 2 ㎛ thick films were annealed at 550°C in H_2S atmosphere. Sulfurization produced 1.02 ㎛ thickness of kesterite CZTS lagers and the composition of Cu: Zn: Sn: S = 2.02: 0.96: 0.92: 4.14. The CIS nanoparticles were synthesized with CuCl, $In(NO_3)_3$ and thiourea in ethylene glycol. The synthesized CIS nanoparticles exhibited single phase Zinc-blend XRD peaks. The heat treatment at 550°C in H_2S atmosphere of CIS led to chalcopyrite structure and the composition of Cu : In : S = 1.01 : 1.02 : 2.11.

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Anion-exchange synthesis of $CuInS_2$ polycrystalline in aqueous solution at room temperature

이상남 정덕영* 남혜진[1]

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Chalcopyrite $CuInS_2$(CIS_2) has been promising materials for highly efficient thin film solar cells. However, vacuum-based processes for making of these absorber layers raise cost and technical limitation on the fabrication of PV devices. We report here in the non-vacuum syntheses of precursor materials for CIS_2 absorber layer and characterized properties. Advantages of hydroxide-based precursor synthesis were stability of air atmosphere and easy of synthesis. Metal hydroxide precursors for $CuInS_2$ thin films were synthesized by using a co-precipitation method. We prepared mixed metal hydroxides containing Cu^{2+}, In^{3+} with various molar ratios and added an aqueous NaOH solution at room temperature. After dispersion of solid metal hydroxide precursors in ethanol, the colloidal solution was mixed with the aqueous Na_2S. In other words, it can be a way of synthesizing CIS_2polycrystalline in aqueous solution at room temperature. The CIS_2 precursor was synthesized by anion exchange reaction and heat treatments crystalline powder. The prepared CIS_2 were characterized by Scanning Electron Microscopy(SEM) and X-Ray Diffraction(XRD)

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Structural transformation of exfoliated $Co(OH)_2$ without surfactant and synthesis of $Co(OH)_2$-graphene oxide nanocomposites

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We synthesized α-$Co(OH)_2$ powder by gas transfer method. Petri dishes containing an aqueous solution of 0.1M $CoCl_2$ and one containing a dilute solution of NH_4OH were placed in the same enclosed container. The reactions were carried out under ambient condition. After 6h, cobalt hydroxide was grown perpendicular to the surface with layered thickness of 50nm. Also it were successfully exfoliated into β-$Co(OH)_2$ nanosheets directly by using stirring and heating in formamide simultaneously from α-$Co(OH)_2$ -chloride. Using only one-step exfoliation without applying surfactants and transforming α-$Co(OH)_2$ nanosheets to β-$Co(OH)_2$ nanosheets are significant. β-$Co(OH)_2$ nanosheets were self-assembled with graphene oxide sheets through Coulomb interactions. We demonstrated the nanostructures of β-$Co(OH)_2$ and graphene oxide sheet-on-sheet composites by TEM and Raman spectroscopy. These nanocomposites are promising for pseudocapacitor to enable high theoretical capacitance, light weight, and large surface area.

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Nanoporous Transition Metal Dichalcogenides ME_2 (M = Mo, W; E = S, Se) with Layered Crystallinity as Anode Materials for Lithium Ion Battery

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The layered nanomaterials including transition metal dichalcogenides (TMDs) are expected to have great potential in nano-electronics, sensing and energy harvesting. As the layered TMDs can be made into porous structure with structural flexibility, energy devices such as photovoltaics, and capacitors can be envisaged. Furthermore, the layered structures allow ionic or molecular intercalation, suggesting possible applications in lithium ion batteries (LIBs), hydrogen storage, catalysis and electrochemical double layer capacitors. Thus, introduce the mesoporosity to the materials would be very important strategies for the creation of 3-D nanostructures. The mesoporous materials have some advantages as a LIB electrode: highly tunable porosity can easily allow liquid electrolyte diffusion into the bulk of an electrode material, providing fast transport channel for lithium ions and also supplying space for volume change during the charge/discharge processes. The thin pore walls ($_2$ (M = Mo, W; E = S, Se) with developed layered crystalline frameworks for LIBs. The obtained materials exhibit high surface area, ordered meso-structures, and higher lithium capacity than theoretically calculated values based on the conversion mechanism.

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[발표취소] Effect of Various pH values Stability for Blue $CoAl_2O_4$ Pigmentr by Regulation of Shell Starting Material

유리 윤지연[1] 피재환[2] 김유진[*]

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Scattering layer effect of hollow type mesoporous TiO_2 for dye-sensitized solar cell

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성균관대학교 화학과

There have been lots of researches to enhance DSSC performance by developing new sensitizer, electrolyte, and photoelectrode materials, reducing the charge recombination, and so on. Also, for improvement of light harvesting efficiency in photoelectrode, light-scattering effect was investigated. This effect could be introduced by adding a layer with large size particles. Large size particles reflect and scatter the irradiated and/or scattered light from photoelectrode. This reflected light was re-absorbed by dye-sensitizers and generated more charges.Recently, hollow type metal oxides were investigated as light-scattering materials. Hollow shell could not reflect and scatter, but also trap the light inside. It helped charge generation enhanced. If hollow shell have a mesoporous structure, it would have both light-scattering effect and dye-adsorbing ability which is a very important factor on the DSSC performance. In this study, we were synthesized various hollow type mesoporous TiO_2s by using coating and hard template method. Synthesized materials were characterized by X-ray diffraction (XRD), N_2-sorption isotherm for adsorption ability, UV-visible spectrometer for the actual concentration of dye-adsorbed, electron microscopy, diffuse reflectance UV-visible spectrometer, and solar simulation with solar simulator and incident photon to charge carrier efficiency (IPCE.)

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Synthesis and Characterization of New Materials for OTFTs

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We have synthesized a novel polymer, alkoxy naphthalene substituted anthradithiophene conjugated polymer, via Suzuki coupling polymerization. The newly designed copolymer is expected to have good mopology and charge carrier mobility due to the anthradithiophene and alkoxy naphthalene with a planar π-π system. Furthermore, long alkyl groups on the naphthalene increase the π-π stacking characteristics through easy interdigitation and can increase the solubility in the common organic solvents such as chloroform, dichlorobenzene, toluene, and THF. The synthesized copolymer was characterized by 13C-NMR, 1H-NMR and gel permeation chromatography (GPC). The thermal properties were determined by thermogravimetry analysis (TGA) and differential scanning calorimetry (DSC). Electrochemical and optical properties of copolymer were studied by UV-visible and cyclic voltammeter (CV) in solution and film.

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High-Performance n-Channel Organic Thin-Film Transistors

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A high-performance naphthalene diimide (NDI)-based conjugated polymer for use as the active layer of n-channel organic field-effect transistors (OFETs) is reported. The solution-processable n-channel polymer is systematically designed and synthesized with an alternating structure of long alkyl substituted-NDI and thienylene-vinylene-thienylene units (PNDI-TVT). The material has a well-controlled molecular structure with an extended π-conjugated backbone, with no increase in the LUMO level, achieving a high mobility and highly ambient stable n-type OFET. The top-gate, bottom-contact device shows remarkably high electron charge-carrier mobility of up to 1.8 $cm^2 V^{-1} s^{-1}$ (I_{on} / I_{off} = 10^6) with the commonly used polymer dielectric, poly(methyl methacrylate) (PMMA). Moreover, PNDI-TVT OFETs exhibit excellent air and operation stability. Such high device performance is attributed to improved π-π intermolecular interactions owing to the extended π-conjugation, apart from the improved crystallinity and highly interdigitated lamellar structure caused by the extended π-π backbone and long alkyl groups.

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Synthesis of Mesoporous Structured Epoxy Resin

LICHENGBIN JINXING 김지만*

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Porous polymeric materials especially have received an increased level of research interest due to their potential to merge the properties of both porous materials and functional group witch in polymers. For example, they have high specific surface area and well-defined porosity, uniform pore diameter, and easy processability. (e.g. Functional porous polymers can be designed), so porous polymeric materials have gained much attention for adsorption, gas separation, and as precursors of nanostructured carbon materials. The past several years have witnessed an expansion of various methods for getting porous polymers used different polymers, including direct template, block copolymer self-assembly, and direct synthesis methods. Each of these methods has its own strength and limitations. Since Goltner et al. first reported that synthesized of polymeric materials using OMS templates, and gain the porous polymeric materials by removal the silica template.[1]Epoxy resins have been commercially developed for more than three fourth century, and have many major industrial applications owing to their attractive characteristics of high tensile strength, excellent moisture resistance, good chemical and corrosion resistance, and excellent dimensional stability. Although many studies have reported the preparation of epoxy resin/silica composite and they exhibited well performances, there has been no report on the synthesis of mesoporous structured epoxy resin so far. In the present work, we employed the normal mesoporous silica KIT-6 with any surface modification as template for obtaining mesoporous structured epoxy resin. [1] C. G. G?ltner and M. C. Weissenberger, Acta Polym., 1998, 49, 704

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Hydrogen Bond-Triggered, Surfactant Free Synthesis of Mesoporous, Silica-Polymer Nanostructured Materials for the Remidation of Environmental Pollutants

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한국기초과학지원연구원 전주센터 [1]한밭대학교 응용화학과

We have developed an alkali-assisted facile strategy for the synthesis of two types of mesoporous silica nanoparticles (MSNPs) i.e. rambutan-like MSNPs (R-MSNPs) and hollow MSNPs (H-MSNPs) using a surfactant-free strategy at room temperature. A cationic polymer (Polyethyleneimine; PEI) with various molecular weight (2-750 kd) were used. The particle sizes were uniform (~150 nm) with easily tunable surface structures by varying the loading volume ratio of Si/PEI (1:1 to 1:5), reaction time, etc. Both types of MSNPs have a high specific surface area (up to 1025 m^2/g) with large pore volumes (17-38 nm). We investigated the removal of pollutants toward possible future use in environmental remediation applications. For example, exhibited promising performances for the removal of heavy metal with high adsorption capacity (q_e), e.g. for Pb = 343.304 mg/g; Hg =289.2644 mg/g and As =75.075 mg/g. In addition, synthesized materials have been applied for the efficient disposal of waste water containing bulky pollutants- like methyl orange (MO) with a high absorption rate (>95%) and for removals of toxic microcystin-YR (100μg/L) over 97%. Additionally, high loading capacity of gold-NPs offered excellent catalytic activities for the reduction of nitrophenol.

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Simple Synthesis and Luminescent Properties of Poly (9-(3-Vinyl-phenyl)-anthracene) for PLEDs

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가톨릭대학교 화학과 [1]Deerfield Academy

Polymer light-emitting diodes (PLEDs) have attracted much attention from academia and industry field because of their various applications such as large area flat-panel displays and lightings. In this paper, we suggest new blue emitting polymer based on anthracene, Poly (9-(3-Vinyl-phenyl)-anthracene) (PVPA). From NMR data, vinyl group protons were disappeared and aromatic protons showed broad proton peaks because of polymer characteristics. PVPA had film property well and it exhibited vivid PL maximum values of 431, 455, 482 nm and broad PL spectrum. Three dopants for green, red, yellow were used to PVPA, all energy transfer was happened well. By using rubrene dopant of yellow emission, doped film provided white PL.

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The comparative study of VO_2 nanoparticles synthesized by the hydrothermal reaction of V_2O_5 and the thermolysis of vanadyl ethylene glycolate

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부경대학교 화학과 [1](주)마프로 기술연구소

Monoclinic Vanadium dioxide(VO_2) is a thermochromic material of which N-IR absorption property changes due to thermal phase transition. Several synthetic methods of VO_2(M) have been reported and many efforts have been devoted to reduce the transition temperature of the material because of its wide practical applicability. Among them the hydrothermal reaction of V_2O_5 with oxalic acid and the thermolysis of vanadyl ethylene glycolate(VEG) are most promising ways to synthesize VO_2(M) in the practical aspects of cost and easiness. In this study we have thoroughly investigated the relative properties of VO_2(M) synthesized by the two different methods. Their changes of phase transition property and morphology due to the reaction control factors such as concetration, time and temperature were studied.

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Co(bpy)$^{2+/3+}$ Redox Couple for Flexible Dye-Sensitized Solar Cells

윤용태 김영일*

부경대학교 화학과

Despite of the high performance of I^-/I_3^- redox couple for dye-sensitized solar cells (DSSCs), it has a few drawbacks including its high corrosive power to metal, relatively high visible light absorption and complex two-electron process. For these reasons, several alternative redox mediators have been extensively studied and the cobalt polypyridyl complexes seemed to be promising among them.Co(Ⅱ) and Co(Ⅲ) trisbipyridyl complexes were synthesized and their electrochemical properties were characterized with several electrodes and solvents. Co(bpy)$^{2+/3+}$-employed flexible DSSCs were fabricated and comparatively studied with variations of electrolyte concentration, types of solvent, amount of additives and types of dyes in order to maximize the power conversion efficiency of the cell.

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Controlling pore size distribution of halloysite manipulating its pH dependent property

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The nanotube structure of halloysite has led to increased interest in its applications as nanoreactors or nanotemplates, catalysts, and capillaries. Since many cases of the applications make use of the lumen of the halloysite, it is important to control the effective lumen size or diameter. The simplest method to do this is to control the pH of the system, because the functional groups of the external or internal surface of the halloysite can readily be affected by changing the pH, thus gives different aggregation/dispersion properties which can increase or decrease the effective lumen volume or diameter. We used two different system, untreated halloysite and carboxylate-modified halloysite. They showed different pH dependence; untreated halloysite showed good dispersibility only at basic condition, but carboxylate-modified halloysite dispersed well at both acidic and basic conditions.

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Synthesis of new nanostructured titanium dioxide-perovskite hybrids via exfoliation and reassembling route

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Because synergetic effect could be derived from a combination of different nanomaterials, the nanohybrid materials through the lattice engineering have received special attention in scientific and industrial fields. In this regard, we have tried to synthesize TiO2/perovskite nanohybrids by using exfoliation and reassembling route. First of all, the colloidal nanosheets with perovskite structure were prepared via soft chemical exfoliation. On the other hand, the titanium dioxide nanosol with average size of 1 nm was synthesized by the hydrolysis of titanium precursors. Then, the obtained colloidal suspension of exfoliated perovskite and titanium dioxide nanosol were reacted to synthesize titanium dioxide-perovskite nanohybrids. The resulting nanohybrids were analyzed by powder X-ray diffraction (XRD), scanning electron microscopy (SEM), transmission electron microscopy (TEM) and UV-vis diffuse reflectance. According to XRD, SEM and TEM results, titanium dioxide nanoparticles were intercalated into the interlayer of layered perovskite. Furthermore, the band gap of hybrid materials can be tuned by the present hybridization, which was confirmed by UV-vis diffuse reflectance. These results showed that physic-chemical properties of nanohybrids could be effectively modified by hybridizing layered perovskites and titanium dioxide nanoparticles.

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Medium Ion Energy Spectroscopy (MEIS)를 통한 양자점의 원자 분포 확인과 광학적 특성에 미치는 영향 연구

구자정 이진규*

서울대학교 화학부

다양한 구조를 가지는 것으로 제안된 양자점의 구조 연구는 kinetic study, 합성방법, 반응 mechanism, 광학적 특성 등을 통하여 설명 되어왔으나, 작은 크기로 인하여 내부 구조를 직접적으로 정확히 밝히지는 못하여 왔다.이 연구에서는, CdSe, CdSe/ZnS core/shell structure 의 양자점과 CdSe 와 ZnS 의 화학적 조성이 core 에서부터 shell 까지 gradiation 을 이루며 alloy structure 를 이룰 것으로 예상한 양자점 (Gradient structure 양자점)을 합성하여 광학적인 특성을 알아보고, 이들의 내부구조를 Medium Energy Ion Scattering (MEIS) 장비를 통하여 측정 후, 다양한 모델로 시뮬레이션 하여 core, core/shell, alloy 구조를 원자의 분포 분석을 통하여 비교?확인하여 보았다. 그 결과, gradient structure 양자점의 경우, CdSe core 부분과 ZnS shell 사이에 CdZnSSe 형태의 alloy structure 를 이루고 있는 것을 직접 확인할 수 있었다.

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Preparation of Non-stiochiometric Cu-Mn Oxide Catalyst by Intercalation Method using Basic Copper Salts

이희숙 김세희 한양수*

(주)세일에프에이 연구소

Basic copper acetate, $Cu_2(OH)_3(OCOCH_3).H_2O$ has a layer structure of the botallackite type. The acetate ions are located between the positively charged copper hydroxide layers and exchangeable with various anions including MnO_4^- ion. The MnO_4^- exchanged product has a composition of $Cu_2(OH)_3MnO_4$, though the XRD pattern of this compound could not be indexed on the basis of an usual unit cell derived from a simple botallackite-type structure. Thermal decomposition of the intercalated compound of $Cu_2(OH)_3MnO_4$ at around 450 ℃ resulted in the amorphous Cu-Mn oxide, subsequently crystallized to $CuMn_2O_4$ and CuO on further heating. The amorphous and non-stoichiometric copper-manganese oxide catalyst exhibited excellent catalytic effect in the conversion of CO to CO_2 at 30 ℃.

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Preparation of Porous Mineral (Scoria) by a Simple Acid Leaching and its Gas Removal Efficiency

이희숙 김세희 한양수*

(주)세일에프에이 연구소

Mineral powder (Jeju Scoria) was bleached simply by treating with acidic solution to obtain porous mineral powder. Acid treatment conditions such as acid concentration (4~8 N), temperature (25~80 ℃) and period (4~12 h) were varied systematically to compare the effect on porous structure and mineral composition. Acid treated minerals exhibited increased surface area and pore volume compared with those of raw mineral powder. XRF analysis showed that iron and magnesium species were mainly removed during the acid leaching process. Such prepared porous scoria powders also showed enhanced CO removal efficiency. Further increase in CO gas removal efficiency could be obtained by heat treatment of bleached scoria powders under reducing (H_2/N_2) atmosphere.

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Effect of Cation/Anion Co-substitution on the Visible Light Photocatalytic Activity of Self-Assembled CdS-Layered Titanate Nanohybrids

이장미 황성주[1,*]

이화여자대학교 화학나노과학부 [1]이화여자대학교 화학·나노과학과

We are successful in synthesizing cation/anion-co-substituted CdS-Ti(5.2-x)/6Rhx/2O2-yNy nanohybrids via an electrostatically-derived self-assembly between Rh/N-substituted layered titanate nanosheets and CdS quantum dots (QDs). The replacement of Ti with Rh and that of O with N in the layered titanate phase are commonly evidenced by powder X-ray diffraction, UV?vis spectroscopy, and zeta potential measurements. Field emission-scanning electron microscopy and energy dispersive spectrometry clearly demonstrate the homogeneous distribution of Rh and N in the entire region of layered titanate nanosheets. In terms of electrostatic interaction, the positively-charged CdS QDs with the particle size of ~2.5 nm can be immobilized on the surface of negatively-charged Ti(5.2-x)/6Rhx/2O2-yNy 2D nanosheets, leading to the formation of mesoporous stacking structure with expanded surface area. A strong electronic coupling between these two components is confirmed by diffuse reflectance UV?vis spectroscopy and photoluminescence spectroscopy. The present CdS-Ti(5.2-x)/6Rhx/2O2-yNy nanohybrids exhibit much higher photocatalytic activity for visible light-induced H2 evolution, which is superior to those of the unsubstituted CdS-TiO2 nanohybrid and the precursor CdS QDs. This result provides strong evidence for the beneficial role of the co-substitution of Rh and N in improving the photocatalytic activity of titanate nanosheet-based hybrid materials.

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Improved Electrode Functionality of Multicomponent Co-Al-LDH/Reduced Graphene Oxide/Layered MnO_2 Nanocomposites for Supercapacitor Application

구태하 황성주*

이화여자대학교 화학·나노과학과

Multicomponent Co-Al-layered double hydroxide (Co-Al-LDH)/graphene/layered MnO_2 nanocomposite can be synthesized by the crystal growth of Co-Al-LDH crystallites in the presence of the mixture colloidal suspension of graphene oxide (G-O) and layered MnO_2 nanosheets under refluxing condition. Due to the similar chemical nature and surface charge, both the G-O and layered MnO_2 nanosheets can form stable colloidal suspensions. Since both the nanosheets possess negative surface charge, the cobalt ions are readily adsorbed on the surface of these nanosheets, which is followed by the growth of the Co-Al-LDH crystallites. Simultaneously the precursor G-O is reduced to reduced graphene oxide (rG-O) with the help of urea. The formation of Co-Al-LDH phase is confirmed by X-ray diffraction analysis with good dispersion of rG-O and layered MnO_2 nanosheets in the nanocomposite matrix. Field emission-scanning electron microscopy and energy dispersive spectrometer analysis indicates the formation of porous stacking structure and the homogeneous hybridization of all the components. The multicomponent Co-Al-LDH/rG-O/layered MnO_2 nanocomposites show promising electrode performance with large specific capacitance and excellent cyclability, which are superior to those of the pristine Co-Al-LDH and the binary Co-Al-LDH/rG-O nanocomposite. The present results provide strong evidence for the usefulness of metal oxide nanosheet in optimizing the electrode performance of LDH/graphene nanocomposites.

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Preparation of Cobalt Supported Wrinkled Silica Nanoparticles(WSNs) for Fischer-Tropsch Synthesis

정동욱 문두식 이진규*

서울대학교 화학부

Recently, Fischer-Tropsch(FT) synthesis has been receiving much attention again for the conversion of natural gas, coal, and biomass-derived synthesis gas into liquid, due to the increasing crude oil price and the demand for clean fuels. Cobalt catalysts immobilized on the porous solid support are preferred for the FT synthesis because of their high productivity, high selectivity for linear long chain hydrocarbons, and also low activity in the water-gas shift reaction. However, the sintering of the catalyst can be induced by the harsh temperature and pressure conditions of the FT synthesis and it can reduce catalytic properties such as activity and life time. Herein, we repot the preparation method of cobalt catalysts supported on the hierarchical mesoporous silica nanoparticles with a wrinkle structure (WSNs), Co-WSN, for the FT synthesis. The wrinkle structure can isolate adjacent Co catalysts from each other and prevent them from sintering, and the high surface area of wrinkle structure can significantly increases accessibility of active sites. Detailed conditions for catalyst synthesis in order to optimize the catalytic properties will be discussed.

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[발표취소] SiO_2-Coated Cu_2O nanoparticles are more stable than SnO_2-Coated Cu_2O nanoparticles

유리 윤지연[1] 피재환[2] 김유진*

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Fabrication and Characterization of Zn_2SiO_4:Mn^{2+}nanocrystals by controlled silica shell thickness

유리 윤지연[1] 피재환[2] 김유진[*]

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This manuscript reports the synthesis and characterization of ZnO@Zn_2SiO_4:Mn^{2+} and Zn_2SiO_4:Mn^{2+} using ZnO@SiO_2 nano spheres. The SiO_2-shell thickness of the nano sphere was controlled 20 to 60 nm, and was controlled by selecting the reaction time of the Stober method. Zn_2SiO_4:Mn^{2+} was prepared by addition of Mn^{2+} precursor the ZnO@SiO_2 core-shell and then reacted in aqueous solution. Finally, the reactant was annealed at 1000 °C so that Zn_2SiO_4:Mn^{2+} particles were obtained. The structure, morphology and luminescent property of the synthesized samples were determined by XRD (X-ray diffraction), TEM (transmission electron microscopy) and PL.

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Preparation of graphene via solution phase method using Flavin mononucleotide as surfactant

윤우진 주상용*

연세대학교 화학과

Synthesis of graphene via solution phase is proper method for mass production and high applications. We have demonstrated a method using flavin mononucleotide as surfactant for dispersing and exfoliating a natural graphite in solution. Flavin mononucleotide (FMN), a phosphate analogue of vitamin B2, consists of an aromatic isoalloxazine moiety and a chiral d-ribityl phosphate group. A previous study indicates that the isoalloxazine moiety of FMN forms π-π interactions (~2 eV) with carbon nanotubes and enables dispersing single-walled nanotubes (SWNT) individually. Such binding affinity of FMN can be applied to exfoliating graphene from natural graphite by overcoming van der Waals forces between layers. And the hydrophilic ribityl phosphate group enables dispersion of graphene into aqueous media. Dispersion of graphene was prepared using sonochemical method and ultracentrifugation. The resulting graphene samples were characterized by raman & widefield raman spectroscopy, atomic force microscopy (AFM), X-ray photoelectron spectroscopy (XPS) and transmission electron microscopy (TEM). To investigate electrical properties of synthesized graphene, we have formed conductive films and measured sheet resistance according to the transmittance of film. As a results, few-layer graphene has been synthesized in a clear greenish-dark dispersion, and the synthesized graphene has special features about disorder which suggest that graphene flakes possess nanostructures like ribbon.

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Electrochemical fluorescence switching in the NIR region using an electroactive NIR fluorophore

서석재 김은경*

연세대학교 화공생명공학과

The electrochemical fluorescence (EF) switching in NIR region was realized from a NIR electroactive fluorophore which displays high absorption and emission in NIR region. After careful examination of the relations between the chemical structures of dyes and their optical and electrochemical reactions we could optimize the reversibility of the electrochemical fluorescence from an ionic polymethine dye and could achieve fluorescence modulation in NIR region. The applied potential was controlled precisely to achieve reversible EF switching, by minimizing the dimerization process of polymethine dyes. In an optimized condition, the reversibility of the device was a lot improved to show a cyclability of ~100 cycles. Also, the NIR fluorescence modulation became visible in a switching device by using a visible cut-off filter.

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Phase transformations of rare earth oxychloride in aqueous solution

<u>이병일</u> 변송호*

경희대학교 응용화학과

Unexplored phase transitions of PbFCl-type rare earth oxychlorides (REOCls), where RE = La - Dy, and Y, were closely studied in water. In REOCl-water systems, we have investigated that the equillbria of the rare earh -oxychloride (REOCl), -hydroxychloride ($RE(OH)_5Cl?nH_2O$), and -trihydroxide ($RE(OH)_3$) phases have the interrelationship in water. The systematic phase diagrams for equilibrium were established in sufficient amounts of water. The hydrolysis of REOCl required a special parameter, the dilution ratio factor (D = volume of water/weight of powder), to be used for REOCl - $RE_2(OH)_5Cl?nH_2O$ - $RE(OH)_3$ phase relationships in water at different temperatures. The equilibration of REOCl in solutions of low dilution ratios ($D \leq 0.5$ mL/mg) yielded all three phases depending on the nature of the RE, dilution ratio, and temperature. Interestingly, the addition of Cl^- salt to systems at similar dilution ratios markedly increased the stability of $RE_2(OH)_5Cl?nH_2O$ phases. The present investigation provides systematic phase diagrams for rare earth oxychloride-water systems that can be used as guidelines for the preparation and application of REOCl - $RE_2(OH)_5Cl?nH_2O$ - $RE(OH)_3$ phases in aqueous media.

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Synergistic effect of organic and metalate ions on Eu-doped layered gadolinium matrices for enhanced red emissions

정희진 변송호*

경희대학교 응용화학과

Organic molecules can act as sensitizers for the enhancement of luminescence property. In particular, the carboxylate anions have been reported much more strongly enhanced anions than the sulfonate in the red lumincescence of Eu^{3+}. In this study, we have used meta-vanadate (VO_3^-) and oleate anions as antenna for energy harvesting and organic sensitizers, respectively, to enhance red emission on LGdH:Eu matrix. Stable luminescent colloidal solution was prepared by simply mixing oleate exchanged form (LGdH:Eu-Ole) with meta-vanadate ions in chloroform. When we added aqueous $NaVO_3$ solution to the colloidal solution, small amount of VO_3^- ions were adsorbed on the surface of LGdH:Eu-Ole nanosheets. After adsorption reaction of meta-vanadate, the structure of LGdH:Eu-Ole was maintained. Interestingly, the red emissions of the meta-vanadate adsorbed LGdH:Eu-Ole was extremely enhanced than that of meta-vanadate adsorbed LGdH:Eu or LGdH:Eu-Ole materials. This synergistic effect by oleate and meta-vanadate ions on the surface of LGdH:Eu led to efficient energy transfer from the ligand-to-metal charge transfer (LMCT) band of meta-vanadate to Eu^{3+} ions as well as highly enhanced f-f transitions, resulting in the bright red emission under 254 nm UV irradiation. The meta-vanadate adsorbed LGdH:Eu-Ole was readily exfoliated in chloroform to form a transparent colloidal solution. The luminescent colloid of meta-vanadate adsorbed LGdH:Eu-Ole showed potential utility as a new class of multimodal probe for biomedical applications.

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Recovery behaviors of calcined layered yttrium hydroxychlorides

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경희대학교 응용화학과

Layered rare-earth hydroxides (LRHs), composed of positively charged rare-earth layers and exchageable inorganic/organic anions in interlayer, are structurally similar to layered double hydroxides (LDHs). Particularly, the recovery ability of LDHs after annealing (from mixed oxide to essentially layered structure), called ‘memory effect’, have an advantage for loading more molecules into interlayer space. In this study, we have investigated recovery behavior of calcined layered yttrium hydroxychlorides, which is different from those of LDHs under specific conditions. By rehydration and rehydroxylation in aqueous solution containing organic and inorganic anions, the intralayer structure of LYHs calcined up to 600°C can be reconstructed to recover the intercalation ability. This calcinations temperature capable of after-reconstruction is quite high compared to those of classical LDHs. High thermal stability and reconstructability would provide the LRHs family, including LYHs, with many advantages for high temperature applications.

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Luminescence quenching effect of CrO_4^{2-} ion on layered rare earth matrices

이진미 정희진 변송호[*]

경희대학교 응용화학과

Water pollution due to heavy metals is caused by several sources such as metal plating, mining, and painting, and also by agricultural sources such as fertilizers and fungicidal sprays. The toxic heavy metals, when present in the water more than the permitted limit, become injurious to the health. With regard to heavy metal pollution, there have been growing interests in the development of new materials to remove toxic metal ions even in low concentration from the contaminated water. Especially, chromium (Cr) is a highly toxic metal to animals at levels above 0.1 ppm, and it causes allergic dermatitis. In this study, layered gadolinium hydroxychloride matrix containing Tb^{3+} (LGdH:Tb) was applied to detect (trace) amount of chromate ions. The adsorption of chromate anions on LGdH:Tb surface was quickly occurred within a few minutes. Generally, LGdH:Tb has typical Tb^{3+} green light emission due to intra d-f transitions at room-temperature excitation. When only small amount of chromate ions were adsorbed on the layered gadolinium hydroxide, the sharp decrease of the strong green emission of LGdH:Tb was observed. The efficient luminescence quenching effect to Tb^{3+} would provide an effective way to detect and remove (trace) amount of chromate ions from water.

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Fabrication of composite PVA films capable of white radiation

위정헌 이병일 변송호*

경희대학교 응용화학과

Organic/inorganic hybrid composites are increasingly developed for use in applications such as flame retardant materials, gene and drug delivery, catalyst carriers and, possibly most importantly, flexible substrates because they show outstanding flexibility and optical clarity. These applications are enabled by the desire nature of organic/inorganic phases which are synergistically combined to form a homogeneous hybrid network. In this study, we have fabricated composite films with white radiation and demonstrated that the inorganic/polymer hybrid films system formed by layered rare earth hydroxychlorides (LRHs) and poly(vinyl alcohol) (PVA) exhibit highly optical transparency, and also can display versatile photoluminescence (PL) features at rolled or folded shapes. As primary color components to implement white color, calcined-LGdH:REs (RE = Eu, Tb), and LYH:Ce were selected as luminescent materials for red, green, and blue displays in PVA matrix. Because c-LGdH maintains the characteristics layered structure comprising significant amounts of hydroxyl groups after calcinations at 600 °C, highly luminescent c-LGdH:RE (RE=Eu, Tb) was effectively dispersed without extensive condensation and/or aggregation in the hydrophilic PVA matrix. Small amount of the LYH:Ce powder could be also dispersed in PVA and exhibited a strong blue emission. The white emission of LRH/PVA film could be simply tunable by controlling the mixing ratio of different types of c-LGdH:RE nanosheets and LYH:Ce powder. The resulting LRH/PVA film generated an excellent white-light under 254 nm UV irradiation.

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Aqueous solution route for synthesis of $GdVO_4$ nanoparticles

이연혁 정희진 변송호*

경희대학교 응용화학과

Stable luminescent colloidal solution was prepared by simply mixing Eu^{3+}-doped layered gadolinium hydroxychloride (LGdH:Eu) nanosheets with meta-vanadate (VO_3^-) ions in water. In water, the reaction between LGdH:Eu and VO_3^- led to rapid formation of $GdVO_4$:Eu with spindle-like morphology at room temperature. Interestingly, approximately 100 nm sized $GdVO_4$:Eu nanoparticles were well dispersed to form a stable translucent colloidal solution without any stabilizing agent, probably due to remnant hydroxyl groups on the surface of $GdVO_4$:Eu nanoparticles that facilitate the hydrogen bonding with water molecules. The colloidal solution exhibited efficient energy transfer from the ligand-to-metal charge transfer (LMCT) band of meta-vanadate to Eu^{3+} ions as well as highly enhanced f-f transitions, resulting in the bright red emission under the commercial 254 nm UV irradiation. These luminescent colloids of $GdVO_4$:Eu showed potential utility as a new class of multimodal probe for biomedical applications. This simple route without heating process in water can provide a reproducible large-scale synthesis method for preparing of $GdVO_4$:Eu nanoparticles at room temperature.

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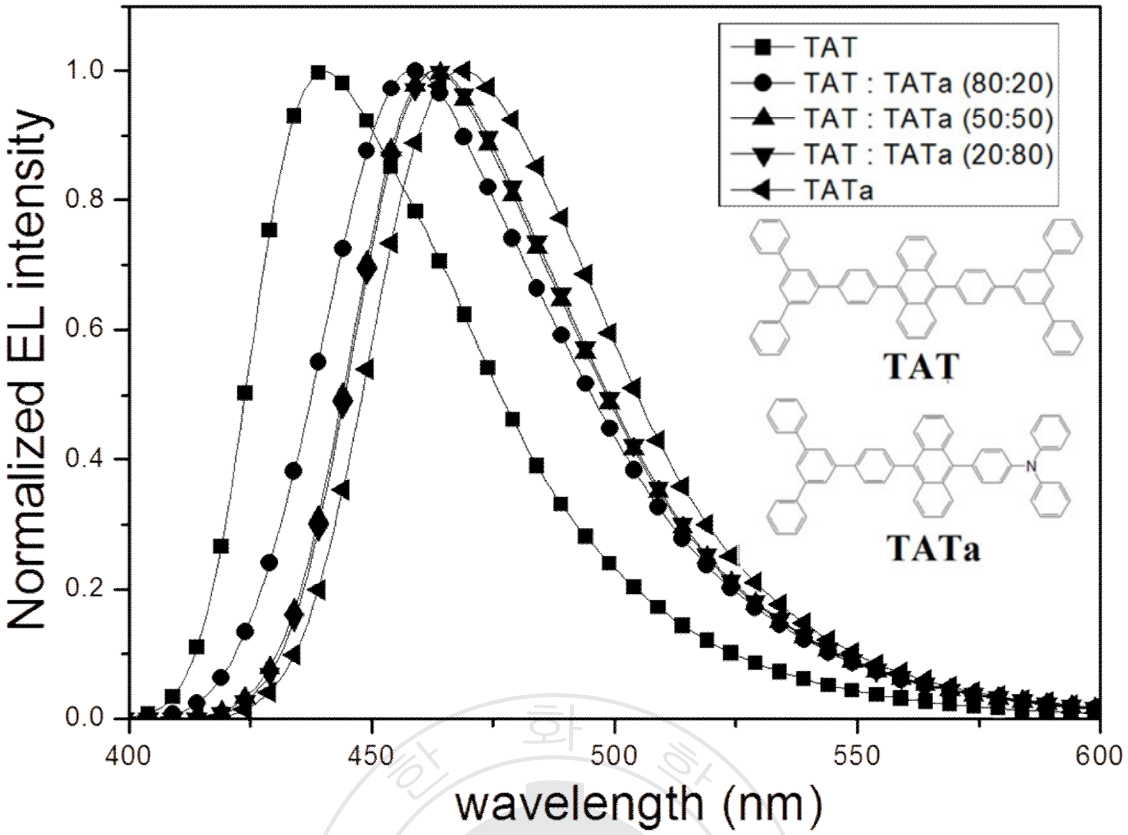
Blue Emission Color Control by Co-Deposition Method Using Blue Materials as Emitting Layer in Organic Light Emitting Diodes

이재현 박종욱*

가톨릭대학교 화학과

In previous paper, we reported new high performance blue emitting materials, 9,10-bis(3",5"-diphenylbiphenyl-4'-yl)anthracene(TAT) and 4-(1'(3',5'-diphenylbiphenyl-4-yl)anthracen-9-yl)-N,N-diphenylaniline (TATa) which have electroluminscence (EL) maximum values of 443nm and 469nm. OLED devices were fabricated and characterized by co-deposited emitters of TAT and TATa with different ratio. EL maximum wavelength was changed from 443nm to 469nm. Further data will be discussed in presentation.


Normalized EL intensity
0.0
0.2
0.4
0.6
0.8
1.0
400
450
500
550
600
wavelength (nm)
TAT
TAT : TATa (80:20)
TAT : TATa (50:50)
TAT : TATa (20:80)
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Direct fabrication of Co(OH)?2 /graphene composites from graphite and their electrochemical property

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아주대학교 분자기술학과 [1]아주대학교 응용생명화학공학부

Co(OH)2 nanosheets on graphene were fabricated from graphite by hydrothermal method. The as-synthesized samples were characterized by transmission electron microscopy (TEM), powder X-ray diffraction (XRD), atomic force microscopy(AFM), cyclic voltammetry(CV), and Barrett-Emmett-Teller (BET) methods.The Co(OH)2 nanosheets on graphene were tested for super capacitors as an electrode material. The capacitve properties of Co(OH)2/graphene nanocomposite displayed better than recent research(960F/g at 10A/g). Additionally, over 85% of the initial specific capacitance value at a cuurent density of 30A/g was retained after 5000cycle charge- discharge operation.

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Fabrication of biosensor for the detection of prostate specific antigen using Au attached multi-walled carbon nanotubes

지성경 이명순 김 돈*

부경대학교 화학과

The purpose of this study is fabrication of a inexpensive, simple and sensitive biosensor using Au attached multi-walled carbon nanotubes (MWNTs). The surface of MWNTs was carboxylated by refluxing in concentrated nitric acid. The carboxyl functional group on the surface was confirmed by FT-IR. The functionalized MWNTs was coated by a coupling agent (EDC and NHSS), gold nanoparticles (~4.5 nm in diameter) and monoclonal antibodies (monoclonal anti-KLK3) of the prostate specific antigen in a phosphate buffered saline. The biosensor could be prepared through a very simple suction filtering of the prepared solution, which contains activated carbon nanotubes with micro-filter paper (0.45 nm pore) and syringe. The electrical resistance of the prepared biosensor (4.7 x 1.3 mm^2 pattern size) could be adjusted 500~1000 ohm with the thickness control. The sensitive of the biosensor to the prostate specific antigen will be discussed.

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Sharp metal to insulator transition in cluster of VO_2 crystals by hydrothermal growth

이명순 <u>지성경</u> 김 돈*

부경대학교 화학과

We prepared high quality VO_2 crystals by a hydrothermal reaction for 3 days at 483 K and successive Ar annealing at 773 K for 5 h. Clusters of the VO_2 crystals show clear insulator-to-metal transition (IMT) and metal-to-insulator transition (MIT) in the measurement of the temperature dependence of electrical resistance. However, transition points shift to the higher temperature along with the number of repeated heating and cooling cycles. The reaction temperature and time for the hydrothermal process are very important to get the high quality VO_2 crystals. The sample prepared at 503 K do not show sharp MIT and IMT and the sample prepared at lower temperature than 483 K have poor electrical contacts between the VO_2 crystals.

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Size Influence of Iron Oxide Nanoparticles(Fe_3O_4) for Magnetic Hyperthermia

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Iron oxide nanoparticles are studied for magnetic hyperthermia treatment and there are many researches about influence of size, frequency of alternative magnetic field, current, and concentration in order to find the optimum size of magnetic nanoparticles. However, most researches used various sized nanoparticles of iron oxide which were prepared by different synthetic methods such as thermal decomposition, coprecipitation, and so on. Therefore, the optimum particle size of magnetic hyperthermia suggested from their results could be affected by the crystallinity and crystal size as well as the magnetic domain size of nanoparticles prepared by different synthetic method and temperature. We have successfully synthesized iron oxide nanoparticles in a wide range of diameters from 22 nm to 140 nm by the same synthetic method of solid-state phase transformation. After the surface modification of iron oxide nanoparticles with polyacrylic acid (PAA) to enhance the dispersibility, time-dependent temperature changes of medium (water solution or Agarose gel) was monitored as functions of nanoparticle size, current level, and frequency of alternative electric field. Based on these data, various sized iron oxide nanoparticles were treated to several cancer cells, and the magnetic hyperthermia effect was investigated.

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Light-triggered drug release from dendrimer-nanorod composite membrane

김기범 박홍열 유동건 박명환*

삼육대학교 화학과

Stimuli-responsive smart materials in optoelectronics, surface coating, storage, sensing and drug delivery have received significant attention in recent times. Especially, stimuli-responsive materials are very important in the field of drug delivery to maintain an effective therapeutic range of concentration-dependent drugs over a specific period of time. We have developed the new on-demand delivery strategy using dendrimer-nanorod composite membranes that can be responded to near-infrared (NIR) irradiation. The stimuli-responsive nanoporous membrane was fabricated by dithiocarbamate (DTC) cross-linking with polyamidoamine(PAMAM)dendrimer and gold nanorod. The photothermal effect of gold nanorod leads to rapid increase in temperature at the surrounding area of the composite membranes, resulting in accelerating the release of drugs in the presence of NIR irradiaton. Scanning electron microscopy (SEM) was used to analyze surface morphology of the fabricated membrane and quantitative release of drugs by NIR irradiation was measured by UV-visible spectroscopy or fluorescence spectroscopy over time.

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Photoresponsive Smart Capsules Formed with Gold Nanorods and Photodegradable Polymer

양수정 박홍열 김기범 유자형[1,*] 박명환[*]

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Biomaterials with stimuli-responsive properties have gained considerable attention over recent years in the field of drug delivery because of difficulty for maintaining an effective therapeutic range of drugs within regions over a specific period time to avoid significant side-effects by overdosing and ineffective treatment from underdosing. Various internal and external stimuli such as pH, temperature, enzymes, ultrasound, light, and electric and magnetic fields are being researched. Among them, light is especially attractive because it can be remotely triggered and applied broad parameters such as wavelength, intensity of light, and time of exposure. Here, we developed the new smart capsules that can be responsed to harmless near-infrared(NIR), triggering release of drugs. The robust capsules were fabricated through crosslinking with gold nanorods and amine functionalized photodegradable polymer using dithiocarbamate(DTC) chemistry at oil-in-water interfaces. The structural formation was examined using optical microscopy, scanning electron microscopy and transmission electron microscopy. The release behavior of drugs induced by exposing NIR to the capsules was analyzed by fluorescence microscopy and ultraviolet-visible spectroscopy.

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Synthesis and characterization of fluorescent nanoparticles for quantitative measurement of hydrogen peroxide

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Reactive oxygen species (ROS), including hydrogen peroxide (H_2O_2) known to generate free radical, has important roles in cell signaling and homeostasis. However, the excessive production of ROS may result in many diseases such as cancer, heart disease, stroke, and neurodegenerative disease. To date, fluorescence analysis in combination with a ROS-sensitive fluorescence probe is generally used as a detection method of ROS. Here, we have synthesized poly(urethane acrylate nonionmer)(PUAN) nanoparticles with the H_2O_2-sensitive fluorophore that is chemically conjugated to the nanoparticle matrix. We measured of H_2O_2 levels quantitatively by estimating ratiometric fluorescence intensity of our H_2O_2-sensing nanoparticles. Our nanoparticles have the potential for 1) multiple sensing of biomolecules of interest, and 2) active targeting to specific cell types such as cancer cells.

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콜로이드 오팔 주형을 이용한 니켈 기공 박막의 전기화학적 제조 및 구조 분석

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한국기초과학지원연구원 강릉센터 [1]강릉원주대학교 화학과 [2]강릉원주대학교 전자공학과

비철금속 소재는 최근 국가적으로 진흥해야할 핵심산업으로 부각되고 있다. 비철금속은 보통 철(Fe) 보다 중량이 가볍고 화합물이 되었을 때, 다양한 광학적, 자기적, 전기적 특성을 보이므로 최근 많은 연구가 진행되고 있다. 본 연구에서는 콜로이드입자가 자기조립된 광결정 조립체를 주형으로 사용하여 전기화학적으로 기공성 니켈(Ni) 박막을 제조하는 연구를 진행하였다. 광결정 조립체 하단에 코팅된 금 나노박막을 전극으로 하여 시간대전류법(chronoamperometry)으로 니켈을 전기화학적으로 환원하여 증착시킨다. 니켈은 광결정 조립체의 입자간 공극에 채워지게되며, 주형으로 사용되는 폴리스티렌 콜로이드 입자를 용매로 제거하여 기공성 니켈 박막을 용이하게 얻을 수 있었다. 본 연구는 시간과 주형 입자 크기에 따라 니켈 박막의 성장거동을 주사전자현미경(SEM)과 X-선 회절 분석(XRD) 결과를 통하여 살펴보았다. 향후 니켈 기공성 박막은 이차전지의 전극으로 활용될 수 있을 것으로 기대된다.

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Photothermal-Responsive Organogels for Small Hydrophobic Therapeutics

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삼육대학교 화학과 [1]충남대학교 분석과학기술학과

Organogels are semi-solid systems, in which an organic liquid phase is immobilized within spaces of the three dimensional networked structure formed by the physical interaction between self-assembled gelator fibers. The thermo-reversible property of the organogels and their high capacity of hydrophobic therapeutics have generated much interest for their use as a drug carrier in the field of drug delivery. Here, we have fabricated the organogels composed of vegetable oils, gelators, gold nanorods, and hydrophobic dyes as model drugs. The use of gold nanorods able to absorb and scatter lights strongly in the range of near-infrared (NIR) enables the organogels to be externally manipulated, triggering release of drugs due to transforming the gels core into oil core by photothermal effect of gold nanorods. The structural formation of organogels was confirmed using optical microscopy and scanning electron microscopy and the photoresponsive behavior was analyzed by measuring the concentration of released drugs from organogels using fluorometer and UV-visible spectroscopy.

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The electrical properties and side-gated field effect transistor of Au nanoparticles attached carbon nanotubes

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부경대학교 화학과

Gold nanoparticles (AuNPs) attached to carbon nanotubes (Au-CNTs) was prepared by a decomposition of $HAuCl_4$ at 503 K and a consecutive carbonization of sucrose at 1173 K within anodic aluminum oxide (AAO) template. The diameter of Au-CNTs ($r_{Au\text{-}CNT}$)was in the range of 40 ~ 250 nm, which corresponded to the channel diameter of the AAO template. The shape and crystallinity of the CNT phase were depended on r_{CNT}).; Highly crystallized and straight shaped CNTs was observed when $r_{Au\text{-}CNT}$> 80 nm, and less crystallized noodle shaped CNTs was observed when $r_{Au\text{-}CNT}$< 80 nm. The crystallinity of the CNT phase was confirmed by the analysis of G and D band in Raman shift and the electrical conductivities measurement of Au-CNTs. The electrical conductivity of highly crystallized carbon phase of an Au-CNTs ($r_{Au\text{-}CNT}$= 250 nm) reached up to ~10^4 S/cm. A side-gated field effect transistor (FET), which assembled by using the Au-CNTs, showed that the Au-CNTs can be a promising candidate for various nanoelectronics.

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Study on a novel synthesis of $MnCO_3$ nanoparticles using supercritical CO_2

권영탁 이상하 조미숙 이영관*

성균관대학교 화학공학과

$MnCO_3$ was synthesized by using supercritical CO_2. The size and uniformity of $MnCO_3$ nanoparticles were controlled by varying temperature and pressure. The conditions for fabrication of $MnCO_3$ nanoparticles were optimized ; 50℃, 120bar, 30min. The prepared $MnCO_3$ was characterized by X-ray diffraction(XRD), scanning electron microscope(SEM), Fourier transform infrared spectroscopy (FT-IR), and brunauer-emmett-teller(BET). The electrochemical properties of $MnCO_3$ were confirmed by cyclic voltammetry (CV). Supercritical CO_2 provide to induce homogeneous $MnCO_3$ nanoparticles.

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A Fluorescence Turn-on and Colorimetric Probe Based on Diketopyrrolopyrrole-Tellurophene Conjugate for Selective Detection of Hydrogen Peroxide and Thiols

MATINDERKAUR 양다슬 최기항 조민주 최동훈*

고려대학교 화학과

In the field of supramolecular chemistry, the development of fluorescent probes for the recognition of biologically relevant species has gained considerable attention. Plenty of dyes are available for the design and synthesis of new fluorescent probes. 4-Diketo-3,6-diphenylpyrrolo[3,4-c]pyrrole (DPP) and its derivatives is one of the emerging dyes in supramolecular chemistry for the development of new fluorescent probes. Hydrogen peroxide (H_2O_2) is one of the main reactive oxygen species produced during the activity of almost all oxidases can lead to diverse physiological and pathological events in aerobic organisms. Any increase in the level of cellular H_2O_2 is associated with the DNA damage, aging and cardiovascular disorders. Therefore, the selective detection and removal of these species from the biological system is an issue of medicinal and ecological importance. Several types of probes are available for the detection of H_2O_2 but there is no report no DPP based probe for its detection. This is the first demonstration based on the design and synthesis of an electron deficient DPP based probe linked with a tellurophene moiety. The probe utilizes the redox properties of the tellurium atom for the selective and sensitive detection of H_2O_2; the presence of which is demonstrated by a fluorescent signal. In addition to fluorescence signal, the probe displayed a color change from light blue to light purple upon oxidation by H_2O_2 in aqueous media. The generated tellurophene-1-oxide may be quickly reduced by glutathione to regenerate the original diketopyrrolopyrrole-tellurophene conjugate.

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Si/MoS2 hybrids as high performance anode materials for lithium ion batteries

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경북대학교 화학과

Recently, Si has been considered as a good anode material for Li-ion batteries because it has very high specific capacity of approximately 4200 mAh/g. Nevertheless it has a major drawback due to poor stability. To overcome such an inherent demerit, new Si/MoS2 hybrid materials are fabricated by exfoliation and subsequent reassembling reaction. The X-ray diffraction and transmission electron microscopy analyses showed that Si particles with an average size of 80 nm were successfully attached onto the surface of the MoS2 layer. The electrochemical performance of the obtained hybrid materials was examined by the charge-discharge experiments. Compared to the specific capacity of the bare Si nanoparticle, the hybrid material exhibited much higher specific capacity of 1600 mAh/g even after 30 cycles. Furthermore, these hybrids had enhanced cyclic performances even at higher current rate. Such results indicated that the present synthetic method could be effectively used for improving the electrochemical properties of anode materials in lithium ion batteries.

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Dibenzothiophene-based host materials for Phosphorescent OLED

강주식 조민주 홍태량 최동훈*

고려대학교 화학과

Because of their high triplet energy and bipolar character, dibenzothiophene (DBT) derivatives have attracted considerable attentions to develop phosphorescent host material. Triplet energy and energy levels of DBT-based host materials can be tuned by introducing donor and acceptor moieties. Substitution positions of donor and acceptor moieties also affect the properties of DBT-based host materials. In this work, we synthesized and characterized the series of DBT-based host materials.

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Near Infrared-Triggered Release System of Polydopamin Nanocomposites

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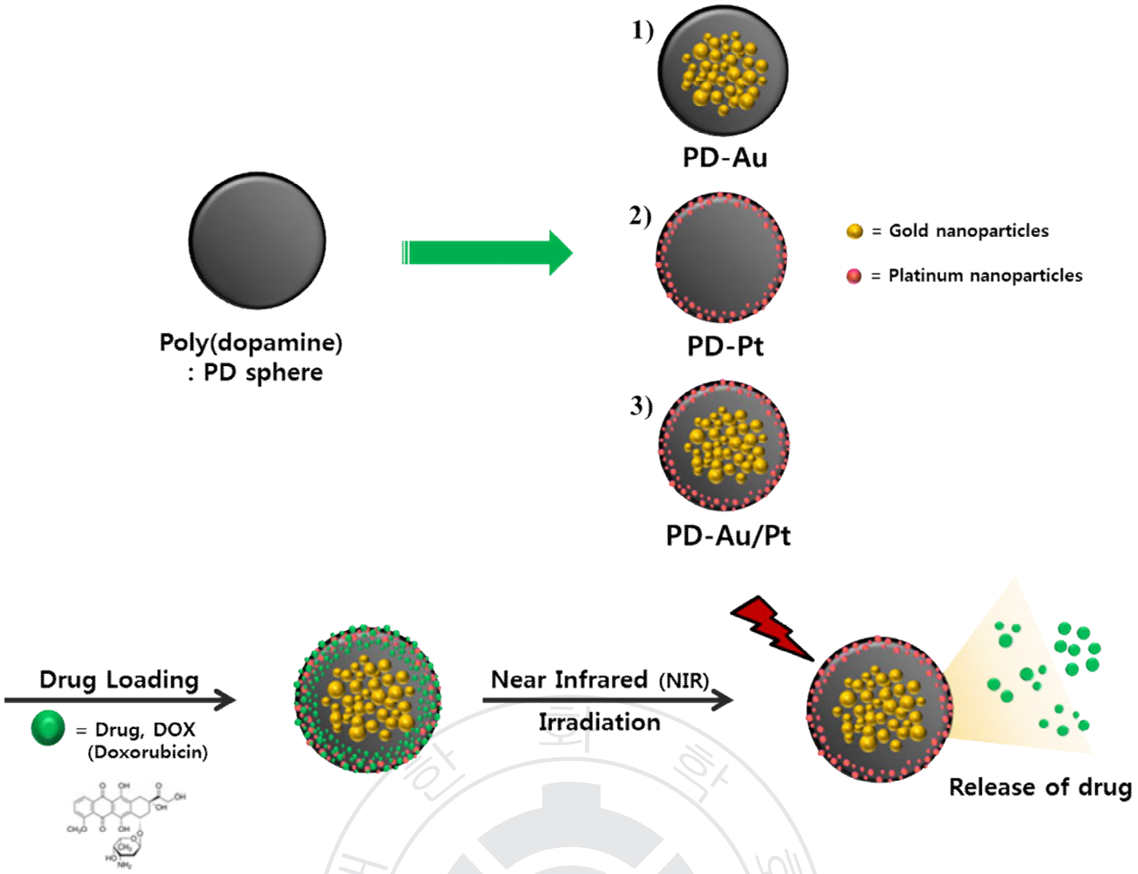
An efficient drug delivery system which releases drugs under near-infrared (NIR) laser irradiation was designed and proposed. A drug carrier is based on the polydopamine (PD) as one of the neurotransmitters, which was used as customized nanoreactors for synthesizing metal nanoparticles (NPs) at the desired site within the PD. Due to the special interactions between metal precursors and the PD, individual NP was selectively positioned within the PD from core to shell. By varying the reaction cycle, it was able to control the loading amount of metal NPs up to almost 95% of the PD particles, which can assist effective release of drug even by short time irradiation of laser. We expect that our system can be used for effective drug carrier capable of controlled release by a minimal stimulus.


1)
PD-Au
2)
PD-Pt
3)
PD-Au/Pt
= Gold nanoparticles
= Platinum nanoparticles
Poly(dopamine)
: PD sphere
Drug Loading
= Drug, DOX
(Doxorubicin)
Near Infrared (NIR)
Irradiation
Release of drug

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Use of Amino Acid as Versatile Dopants for Hetroatom-Doped Graphene

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Graphene, a one atom thick two-dimensional (2D) carbon material arranged in a densely packed honeycomb crystal lattice, has received a great deal of attention in scientific research; graphene has wide-ranging applications in the fields of electronics, sensors, and electrocatalysis due to properties that include being a zero-gap semiconductor and chemically inert. The incorporation of heteroatoms with different electronic characteristics into the structure to predictably alter the electronic properties has great potential in terms of tunable device design and fabrication. Recently, we have developed a simple and efficient method for heteroatom doping in graphene with various dopants. Herein, we report the use of amino acids as versatile dopants for heteroatom-doped graphene.

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π-Extended Diketopyrrolopyrrole-based Conjugated Small Molecules for Solution-processed Solar Cells

홍태량 신지철 엄현아 조민주 최동훈*

고려대학교 화학과

The donor-acceptor (D-A) strategy has been demonstrated to be an efficient approach, in which conjugated electron-rich and electron-deficient units are employed to prepare small molecules. In this work, we designed D-A-D-A-D and D-A-D-D-A-D type molecular structures containing diketopyrrolopyrrole (DPP) and thiophene units for investigating the influence of effective conjugation length on the performance of organic photovoltaics (OPVs) made with ($PC_{61}BM$). So we investigated their electronic or intrinsic properties through theoretical calculation. In addition, absorption spectroscopy, cyclic voltammetry and thermal analysis were performed for characterizing their properties. Finally, we fabricated organic photovoltaics devices with small molecules in combination with $PC_{61}BM$.

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[발표취소] Nitrogen doped activated charcoal as electrocatalysts for the oxygen reduction reaction

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울산과학기술대학교(UNIST) 친환경에너지공학부 [1]울산과학기술대학교(UNIST) 에너지공학부

발 표 취 소

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Double Helix-like Ag_2CO_3/Ag_2O Rods for Sunlight-driven Photocatalyst and NIR-Triggered Drug Delivery System

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The ellipsoidal or rod-like Ag_2CO_3 nanostructures were synthesized by a facile precipitation reaction in the presence of PVP. The resulting Ag_2CO_3 nanostructures were transformed into the Ag_2CO_3/Ag_2O nanostructures by controlled heat treatment. During the heat treatment, both of Ag_2CO_3 nanostructures were changed into double helix-like microrods by fusion of individual nanostructure. Double helix-like Ag_2CO_3/Ag_2O microrods (DHAgMRs) with high specific surface area exhibited a strong absorption band in the range of visible (vis) to near infrared (NIR) regions, meaning that the catalytic property of the DHAgMRs can be activated by the sunlight. After synthesis of mesoporous SiO_2 layer on the DHAgMRs, we expect that the resulting DHAgMR/SiO_2 can be used as a drug delivery carrier triggered by NIR irradiation as well.

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Surface-modified and Cytotoxicity Assay of monodispersed Gold Nanoparticles

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Nanoparticles (NPs) have unique physicochemical properties such as optical activities, bio-stabilities, and flexibilities of surface modification. Nanoparticles became a promising platform for biomedical applications, for example imaging, biosensing, phototherapy and drug/gene delivery. While the applications of NPs for biological systems have been the focus of interest, the fundamental understanding of the interactions between NPs and their target cells, such as plasma membrane, nuclear compartments, organelles and cytoplasm, remain largely unexplored. In this study, we produce a series of surface charge-controlled gold Nanoparticles (AuNPs) ranging in size from 20 to 100 nm by sequential ligand exchange (SLE). Citrated-capped AuNPs with various sizes were modified by thiol ligands (positively charged, negatively charged and neutral). Surface-modified AuNPs were characterized by using analytical tools such as dynamic light scattering (DLS), zeta potential, UV-Vis spectroscopy and existed in monodispersed form. The effect of surface charge and size of AuNPs on cellular toxicity was evaluated by standard MTT assay, tryphan blue assay, cell migration assay and colony forming efficiency (CFE) assay using mammalian cell lines. Because the positively charged AuNPs penetrate better into plasma membrane compared to other NPs, it is probably exhibited extra ordinary cytotoxicity. To better understand the mechanism of NPs-cell interactions, a systemic study of cellular toxicity is essential.

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Synthesis of pliable and osteoblast proliferation stimulating methacrylate resin for potential orthopedic usage

배효근 황동수[1,*]

포항공과대학교 시스템생명공학부 [1]포항공과대학교 환경대학원

Conventional orthopedic cement consists of mostly methylmethacrylate(MMA), which has been widely used since mid-1940s when the material was first applied in surgical field. In this work, another methacrylate, urethanedimethacrylate(UDMA), analogous to dental adhesive material which is also composed of varied mixtures of different kinds of methacrylates are utilized. 3,4-dihydroxyphenylalanine(DOPA) chemistry inspired from marine mussel adhesive protein is unprecedentedly introduced in this study to showing its potential as surgical cement material. We first synthesized key component from a monomer ‘eugenol’, much cheaper than DOPA, and utilized tetra-mercapto chemical to link DOPA derivative to bulky methacrylate. Micro-tensile test and cell viability test with osteoblast, cell line MC3TC, were done with the material to suggest its potential usage as orthopedic material stimulating osteoblast proliferation unlike conventional cements.

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FeF_3/Reduced Graphene Oxide Nanocomposites as a Cathode Material for Lithium-Ion Batteries

제지운 김종식*

동아대학교 화학과

Lithium ion batteries (LIBs) are one of the most commonly used energy storage systems. The fast growths of mobile device and electric vehicle market have been demanding LIBs with enlarged reversible capacities. FeF_3 is of great interest as an alternative cathode material for commercialized $LiCoO_2$ because FeF_3 has high theoretical capacities of about 237 and 712 $mAh\cdot g^{-1}$ in the voltage range of 2.0-4.5 and 1.5-4.5 V, respectively. In addition, FeF_3 has several advantages of low cost, abundance, and environmental friendliness. However, FeF_3 has drawbacks of its low electrical conductivity and sluggish diffusion of the lithium ions, leading to poor capacity retention and rate performance. In this study, FeF_3/reduced graphene oxide (r-GO) nanocomposites with about 1.7, and 11 wt% r-GO are synthesized by utilizing r-GO as a conductive agent through a vapor-solid (VS) method. The prepared FeF_3/r-GO nanocomposites are thoroughly characterized by XRD, FT-IR, EA, SEM, and TEM. FeF_3/r-GO sample with 11 wt% r-GO exhibit an initial specific discharge capacity of about 174 $mAh\cdot g^{-1}$ at 2.0-4.5 V at 0.1 C rate with a capacity retention of about 86.2 % after 50 cycles. In the wide voltage range of 1.5-4.5 V, the FeF_3/r-GO nanocomposites also shows the improved cycling performances compared to bare FeF_3, delivering the initial discharge capacity over 410 $mAh\cdot g^{-1}$ at 0.1 C rate.

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[발표취소] Solvent-Free Diels-Alder Reaction between Graphite and Maleic Anhydride or Maleimide

서정민 백종범[1,*]

울산과학기술대학교(UNIST) 친환경에너지공학부 [1]울산과학기술대학교(UNIST) 에너지공학부

발 표 취 소

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Nanoporous Gold Conjugated with Doxorubicin for Anticancer Drug Delivery and Photothermal Therapy

강태연 채원식*

한국기초과학지원연구원 강릉센터

Nanoporous gold (np-Au) particles conjugated with anticancer drug (doxorubicin) were synthesized and their anticancer activity was characterized. The nanoporous gold particles were synthesized by using anodic aluminum oxide (AAO) membranes (~70 nm diameter and ~50 um thickness), as templates, and its electrochemical deposition in a mixed solution of 0.08M KAu(CN)2, 0.04M KAg(CN)2, and 0.25M Na2CO3 for 30 cycles by pulsed chronopotentiometry. And then, the fabricated np-Au particles were thiolated with dual functional chemicals and subsequently combined with doxorubicin. We will report the doxorubicin release rate and the effect of anticancer treatments for np-Au conjugated with doxorubicin in vitro and in vivo, respectively, by visible-NIR photothermal therapy.

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Fabrication of Reduced Graphene Oxide-TiO_2 Freestanding Film for Supercapacitor Applications

김진수 홍종달*

인천대학교 화학과

Over the past few years, there is an increasing interest in designing high-performance supercapacitors using graphene materials. Graphene has become one of the most promising carbon materials for supercapacitor due to its exellent conductivity and high surface area. However, the restacking of graphene sheets has restricted the performance of graphene based supercapacitors. In our study, a binder-free reduced graphene oxide-TiO_2(RGO-TiO_2) free-standing paper was synthesized using simple vacuum filtration method followed by thermal reduction at different temperature. The TiO_2 nanoparticles were used to prevent restacking of the graphene oxide sheet. The reduction degrees of the graphene oxide at different annealing temperature were studied using Raman spectroscopy and XPS. The effect of reduction temperature on the electrochemical properties of RGO-TiO_2 papers were investigated using cyclic voltammetry, Galvanostatic charge/discharge test, and electrochemical impedance spectroscopy. The RGO-TiO_2 electrode heated at 600℃ exhibited highest capacitive performances with a maximum specific capacitance of 263 F/g at 1 A/g in 1M Na_2SO_4 aqueous electrolyte using a 3-electrode set up.

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Carbon Dioxide Capture Properties of Inclusion Composites Composed of Amines and Metal-Organic Frameworks

심재웅 고낙은 김태민[1] 오유진 김자헌[*]

숭실대학교 화학과 [1]숭실대학교

Carbon dioxide capture from a mixed gas (CO_2/N_2 = 15/85) mimicking flue gas has been explored using composites of MOFs and amine molecules. For a practical application in a post-combustion process, dry sorbents should separate carbon dioxide from flue gas with very fast kinetics, at least 8 CO_2wt%/5min at 40°C which is only possible currently through carbamate formation reactions. In this regard, we have prepared a series of composites by simple inclusion of amines in MOFs: for example, PEI or TAEA in MIL-101 or other microporous MOFs. The inclusion behaviors of amines are related to the pore dimensions in their hosts, and in turn, the resulting composites show various capacities dependent on the nature and loading amounts of included amines.

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Structural reorganization of a metastable nanostructure via postsynthetic impurity doping

박종식 이광렬[*]

고려대학교 화학과

Control of the metal-surface binding moiety interaction has served as the main strategy for the preparation of shape-controlled nanoparticles, which have found important applications in catalysis. The composition of alloy nanoparticle could be dynamically varied by understanding the nature of metal-surface binding moiety interaction. The new alloy phase, obtained from regioselective doping of facet-controlled nanoparticles, might in turn exhibit a surface-stabilization behavior which is completely different from that of the original nanoparticle, leading to the stabilization of different facets and to the formation of completely new nanocrystal shapes. Herein we report a novel transformation of a nanosheet structure into a nanotent structure via postsynthetic impurity doping, which can be further modified to form catalytically active heteronanostructures.

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Porous Metal-Organic Coordination Polymer for Carbon Dioxide Capture

홍지수 유래경 최판규 임나래 양진국* 백경수*

숭실대학교 화학과

A porous metal-organic coordination polymer has been prepared by an Ullmann coupling reaction between Cr(III) oxy acetate type monomers, $[Cr_3O(O_2CR)_6](NO_3)$. The crystal structure of the Cr cluster shows that six 2-nitro-4-iodobenzoate ligands connect three oxo-bridged Cr(III) centers to which MeOH molecules are bound. The terminal iodides in the cluster are reactive toward the coupling reagents to give 2,2’-dinitro-1,1’-biphenyl-4,4’-dicarboxylates, which results in a porous and amorphous coordination polymer solid. After reducing the nitro groups, the produced NH_2 groups are reacted with aziridine in a post-synthetic modification manner to give covalently connected pendant alkyl amines. It is stable under atmospheric or acidic conditions, and uptakes carbon dioxide via physisorption or chemisorption.

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Synthesis of B-doped graphene nano-platelets using a solution process and their supercapacitor applications

한종우 이승준 오정훈 박규태 박성진*

인하대학교 화학과

Chemically modified graphene (CMG) nano-platelets have shown great promise in various applications due to their electrical properties and high surface area. Chemical doping is one of the most effective methods to tune the electronic properties of graphene materials. In this work, novel B-doped nano-platelets (borane-reduced graphene oxide, B-rG-O) were produced on a large scale via the reduction of graphene oxide by a borane-tetrahydrofuran adduct under reflux. This is the first report on the production of B-doped graphene nanoplatelets from a solution process and on the use of B-doped graphene materials in supercapacitors. The B-rG-O had a high specific surface area of 466 m^2/g and showed excellent supercapacitor performance including a high specific capacitance of 200 F/g in aqueous electrolyte as well as superior surface area-normalized capacitance to typical carbon-based supercapacitor materials and good stability after 4500 cycles. Two- and three-electrode cell measurements showed that energy storage in the B-rG-O supercapacitors was contributed by ion adsorption on the surface of the nano-platelets in addition to electrochemical redox reactions.

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Solution-based production of carbon-pure graphene nano-platelets

한종우 이승준 오정훈 박규태 박성진*

인하대학교 화학과

We developed a new route for scalable production of carbon-pure graphene-based nano-platelets via treatment of graphene oxide suspensions with ammonia borane at low temperatures without further thermal annealing. The C/O atomic ratio measured by combustion-based elemental analysis is the highest value among published data on graphene-based nano-platelets using solution processes. Chemical analyses also showed that resulting material was highly carbon-pure, and very high electrical conductivity.

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Generation of B, N co-doped graphene nano-platelets using a two-step solution process and catalytic properties for oxygen reduction reaction

한종우 이승준 오정훈 박규태 박성진*

인하대학교 화학과

Chemically modified graphenes (CMGs) show great promise for various applications owing to the feasibility of their low-cost mass production and good solution processability. Recently, hetero-atom-doped CMGs have been suggested as good candidate materials for electrochemical catalysts in oxygen reduction reaction (ORR). In this study, we synthesized B, N co-doped graphene nano-platelets (BN-rG-O) using a two-step solution process with sequential reaction of graphene oxide with borane tetrahydrofuran and hydrazine monohydrate. BN-rG-O exhibits an onset potential of 0.81 V (vs. reversible hydrogen electrode), follows near four electron pathway, and shows excellent stability against methanol poisoning and during durability tests.

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Fabrication of Flexible Free-Standing Films Composed of Vanadium dioxide /Ultra-Large Reduced Graphene Oxide for High Performance Supercapacitors

이명섭 홍종달*

인천대학교 화학과

Various thin film electrodes have been studied as a promising material for energy storage devices such as supercapacitors due to their fast delivery rate, long cycling life and high power density. Here, we report a facile approach to synthesize vanadium dioxide(VO_2) /reduced graphene oxide(rGO) thin film electrode using vacuum filtration. We observed that the different size of GO sheet has substantial influence on the electrical conductivity and electrochemical properties of the VO_2/ rGO film. The VO_2/ rGO films were characterized using Raman spectroscopy, X-ray photoelectron spectroscopy (XPS) and field emission scanning electron microscopy (SEM). The electrochemical performances of VO_2/ rGO films were investigated using cyclic voltammetry (CV), galvanostatic charge discharge and electrochemical impedance spectroscopy (EIS). The VO_2/ rGO films made from larger GO sheets exhibited high electrochemical performances a high conductivity and low sheet resistance of larger scale GO.

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Highly twinned Au-Pt nanocables with enhanced electrocatalytic activity

윤지선 이광렬*

고려대학교 화학과

The one-pot synthesis of highly efficient electrocatalytic 1-D nanostructure of coaxial Au-Pt nanocable, which exhibits numerous twinning boundaries. Combining the core-shell structure and twinning could result in the surface energy elevation, leading to a great improvement in electrocatalytic activity.

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Graphitic carbon nitride-graphene composites by solution process and their photocatalytic activity

오정훈 이승준 한종우 박규태 박성진*

인하대학교 화학과

Graphitic carbon nitride (g-C_3N_4) and its derivatives could be suitable candidates as catalysts or supports for photocatalytic applications. Since carbon nitride is typically made through or condensation of monomers with high temperature and/or high pressure, production of a cost-effective and solution-based process are important. Graphene oxide has a wide range of oxygen functional groups on basal planes and edges and disperses in water as individual single-layered nanoplatelets. These characteristics of graphene oxide could assist production of carbon nitride by the activity of heavily oxidized graphene forms. Herein, composite materials composed of g-C_3N_4 and reduced graphene oxide (rG-O) are produced by a simple reaction between graphene oxide and precursor of carbon nitride (cyanamide) using a solution-based process. During the reaction, g-C_3N_4 and reduction of graphene oxide were produced simultaneously. These composites show good photocatalytic performance for the decomposition of organic dyes (RhB) under one sun solar light illumination.

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Borane-modified graphene nano-platelets as CO2 adsorbents

오정훈 이승준 한종우 박규태 박성진*

인하대학교 화학과

The authors studied the CO_2 adsorption performances of borane modified graphene-based nano-platelets (B-rG-O). B-rG-O powder was fabricated by reacting graphene oxide with a borane-THF adduct and showed good CO_2 adsorption capacity (1.82 mmol/g at 1 atm) as determined using a CO2 isotherm. CO_2 adsorption was attributed to chemisorption and physisorption by B-rG-O confirmed by Fourier transform infrared and X-ray photoelectron spectroscopy.

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Mass production of thermally reduced graphene oxide and

이승준 박성진* 오정훈 한종우 박규태

인하대학교 화학과

Chemically modified graphenes (CMGs) have been intensively studied as a promising candidate in a wide range of industrial applications. Graphite oxide (GO) is the most common starting material to produce various CMGs. Here we warn the research community that residual acetone, a ubiquitous cleaning solvent in the lab, can produce dangerous explosives during the production of GO using standard methods.

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Solid/Solution Two-step Synthesis of the New Molecular Thiophosphate Cluster$Cr_2P_2S_8(NMF)_4$

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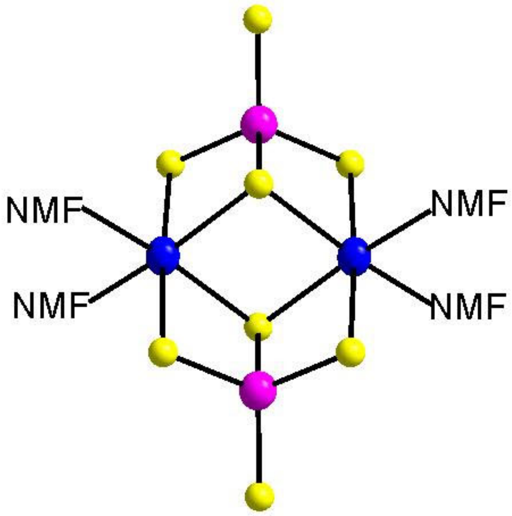
One-dimensional quaternary thiophosphates, $ACrPS_5$ (A=Rb, Cs), have been synthesized via solid state reactions with alkali metal halide fluxes. These compounds are isostructural and they are composed of the one-dimensional anionic infinite chains, ${}^{1}_{\infty}[CrPS_5^-]$ and alkali metal cations. These chains are built up from edge-sharing $[CrS_6]$ octahedra and $[PS_4]$ tetrahedra. Alkali metal ions stay among these chains to stabilize the structure through electrostatic ionic interactions. In order to isolate the anionic species, $CsCrPS_5$ has been dissolved in solvents such as NMF and DMSO. The crystals rapidly dissolved in the solvents. Dark green crystals have been obtained at room temperature from the solution and the crystal structure has been determined by single-crystal X-ray diffraction techniques. The compound has been proved to be $Cr_2P_2S_8(NMF)_4$. Two $[CrS_4]$ units and two $[PS_4]$ tetrahedra are connected by sharing S atoms to form the cluster molecule, $Cr_2P_2S_8$. Each Cr atom is further coordinated by two NMF molecules to complete the octahedral coordination of chromium atoms. We propose that the${}^{1}_{\infty}[CrPS_5^-]$chains dissolved in the solution have been fragmented and the neutral $Cr_2P_2S_8$ cluster and molecular S_8 have been produced by the simultaneous reduction of Cr^{4+} and oxidation of S^{2-} ions.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Full-color-emitting $Eu^{2+/3+}$-doped phosphors using the reaction system of $LaCO_3OH:Eu^{3+}$-Al_2O_3-Eu_2O_3

이민호 최연희 정우식*

영남대학교 화학공학부

The phosphor powders obtained by calcining a mixture of $LaCO_3OH:Eu^{3+}$ and Al_2O_3 in a reducing atmosphere exhibited orange (593 nm) and blue (460 nm) emission bands. The intensity ratio of orange to blue emission bands can be tuned by varying the ratio of $LaCO_3OH$ to Al_2O_3 and temperature. The green (525 nm) emitting phosphor powders were also prepared by the reaction of Al_2O_3 and Eu_2O_3 under a reducing gas flow. Full-color-emitting phosphors using the reaction system of $LaCO_3OH:Eu^{3+}$-Al_2O_3-Eu_2O_3 showed an intense white emission.

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[발표취소] Direct Synthesis of BCN Graphene *via* modified Wurtz reaction

정선민 백종범[1,*]

울산과학기술대학교(UNIST) 친환경에너지공학과 [1]울산과학기술대학교(UNIST) 에너지공학부

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A report on the risk during the production of graphite oxide

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인하대학교 화학과

Mass production of graphene-based materials, which have high specific surface area, is of importance for industrial applications. Herein, we report on a facile approach to produce thermally modified graphene oxide (TMG) in large quantities. We performed this experiment with a hot plate under environments that have relatively low temperature and no using inert gas. TMG materials showed a high specific surface area (430 m2g-1). Successful reduction was confirmed by elemental analysis, X-ray photoelectron spectroscopy, thermogravimetic analysis, and X-ray diffraction. The resulting materials might be useful for various applications such as in rechargeable batteries, as hydrogen storage materials, as nano-fillers in composites, in ultracapacitors, and in chemical/bio sensors.

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Various Li Stoichiometries Induced by Partial Substitutions of Ti with Ta in the Li2Ti?2(PO4)3 System

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Lithium metal phosphates, $Li_{2\pm x}M_2(PO_4)_3$(M=V), have been widely investigated as materials for secondary batteries. It has been reported that the amount of Li can be adjusted in accordance with the oxidation states of metals (M), and Li occupancies are profoundly related to the ionic conductivity. In attempts to control the amount of Li ions by using various metals with different oxidation states, we were able to find new members of this family with non-stoichiometric Li and we report here the synthesis and structural characterization of the mixed-valent compounds, $Li_{2-x}(Ti_{1-x}Ta_x)_2(PO_4)_3$ ($0 \le x \le 0.1$). The framework of the title compounds is the same as that of the previously reported $Li_{2.72}Ti_2(PO_4)_3$ phases (Wang & Hwu, 1991) and the framework is built up from corner-sharing TiO6 octahedra and PO4 tetrahedra. The Li^+ ions are located on one crystallographic position in the vacancies of the framework. They are surrounded by four O atoms in a distorted tetrahedral coordination. In this study, correlation between Li contents and metal substitution will be discussed. The stoichiometry of Li ions in this space can be adjusted by the sum of the oxidation numbers of each metal. The classical charge valence of the compound should be described as $Li_{2-x}([Ti^{3+}]/[Ti^{4+}]_{1-x}[Ta^{4+}]_x)_2(PO_4)_3$.

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Surface-enhanced Raman scattering with Ag flower-like Nanoparticles

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창원대학교 화학과

Raman spectroscopy is a powerful technique to detect and analyze the chemical compounds. However, the poor signal intensities from Raman scattering is the main issue for detecting the analytes at its low concentration. To overcome this problem, surface-enhanced Raman spectroscopy (SERS) had been proposed.Surface-enhanced Raman scattering has been intensely researched for many years as a great potential technique for ultra-trace detection. The enhanced Raman scattering of molecules adsorbed on rough metal surface. The metal surface serves as a highly sensitive detection tool. The mechanism based on the charge transfer between the molecule and adjacent surface. Therefore, the shape of metal will decide the effect of SERS. In this study, Ag nanoparticles with different size and morphologies were synthesized by simple methods from AgNO3, ascorbic acid in aqueous. The SERS effect was investigated using Ag flower-like with some analytes.

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유기물 기반 태양전지 응용을 위한 전도성 고분자 PEDOT 층의 전도성 향상에 대한 연구

황기환 주동우 부진효*

성균관대학교 화학과

대표적 conducting polymer 의 하나인 PEDOT 은 전극으로 쓰이기에는 전도성이 매우 낮다는 단점이 있어, 아직까지 전극으로 사용되기에는 어려움이 있다. 이에 본 연구에서는 기본적인 알콜을 활용하여 Dipping treatment 를 했을때의 PEDOT 박막의 전도성 변화에 대하여 연구를 진행하였다. 전체적으로 PEDOT 박막의 전도성이 매우 큰 폭으로 향상되는 결과를 보였다. 아울러 사용된 알콜은 메탄올, 에탄올, IPA 를 이용하였으며 carbon cahin 이 가장 짧은 알콜인 메탄올을 사용하였을때 가장 큰 전도성 향상이 있었음을 확인하였다. 이때 박막의 특성을 특정하기 위하여 4-point probe, RAMAN spectroscopy, FE-SEM, AFM 을 사용하였다.

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Synthesis and structure of new quarternary thiophosphates, $Cs_3Ta_2PS_{12}$

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During searching for new soluble inorganic polymers composed of Ta, S and P, we have found a new quarternary tantalum thiophosphate, $Cs_3Ta_2PS_{12}$. This compound is synthesized by the reactive halide-flux technique and their crystal structure has been determined by single crystal X-ray diffraction techniques. The title compound can be described as one-dimensional and the anionic polymer chain structure, $^1_\infty[Ta_2PS_{12}]^{3-}$ is consisted of pentagonal-bipyramidal TaS_7 and tetrahedral PS_4 units. Two TaS_7 units are fused to form the dimeric $[Ta_2S_{11}]$ blocks and these blocks and PS_4 units are connected to complete the chain, $^1_\infty[Ta_2PS_{12}]^{3-}$. Finally the $^1_\infty[Ta_2PS_{12}]^{3-}$ chains are stabilized by the Cs^+ ions through electrostatic ionic interactions. The classical charge balance of the compound can be represented by $[Cs^+]_3[Ta^{5+}]_2[P^{5+}][S_2^{2-}]_3[S^{2-}]_6$. UV-Vis absorption spectrum data of the title compound show that band gap is around 2.48 eV.

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Synthesis and Photocatalytic Acitivity of Ru Nanoparticles Supported on Silica Magnetic Microspheres

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창원대학교 화학과

Green chemistry, also called sustainable chemistry, is a philosophy of chemical research and engineering that encourages the design of products and processes that minimize the use and generation of hazardous substances. Green catalysis is a subchapter of green chemistry and probably the most important one. We here report the synthesis, characterization and photocatalytic performance of recoverable ruthenium (Ru) supported on silica coated magnetic microspheres (Fe3O4@SiO2@Ru). The superparamagnetic Fe3O4@SiO2 with well-defined core/shell nanostructure has been synthesized via in situ surface polymerization method. The negatively charged Ru nanoparticles have been effectively assembled onto the positively charged surface of the as-synthesized Fe3O4@SiO2 core/shell microspheres via electrostatic attraction. As-prepared Ru catalysts were characterized by transmission electron microscopy (TEM), scanning electron microscopy (SEM), powder X-ray diffraction (XRD) and Fourier Transform Infra Red (FT-IR) spectroscopy, thermogavimetric analysis (TGA), X-ray photoelectron spectroscopy (XPS) and vibrating sample magnetometry (VSM). The percentage of Ru in Fe3O4@Ru nanocatalysts is obtained by inductively coupled plasma atomic emission spectroscopy (ICP-AES). The synthesized supported Ru catalysts was successfully applied for photocatalytic activity on organic pollutants. The central Fe3O4 cores are superparamagnetic at room temperature with strong magnetic response to externally applied magnetic field, thus providing a convenient means for separating the catalyst from solution. Keywords: Green synthesis, Fe3O4@SiO2 microspheres, Ru nanoparticles, Catalytic applications.

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[발표취소] .

김하영 김성진*

이화여자대학교 화학과

발표취소

본 논문은 발표취소된 논문입니다.

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Solvothermal Synthesis of Lanthanum-doped PbTe Nanoparticles and Their Thermoelectric Properties

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Here we report a simple synthetic method to prepare Lanthanum-doped PbTe nanoparticles via one-pot solvothermal bottom-up approach by using lanthanum(III) acetate hydrate as La precursor. Synthesized La-doped PbTe nanoparticles are characterized by using HR-TEM, EDS, and XRD. The La doping levels can be readily controlled by varying initial concentration of La precursor relative to Pb precursor. The effect of the dopant concentration on the crystal structures were studied with ICP-AES analysis and Rietveld refinement. Furthermore, La-doped PbTe nanostructured bulk pellets with various La doping levels are prepared by hot-pressing process, and their thermoelectric properties were investigated in the temperature range from 300K to ~750K.

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Synthesis of Ce^{3+}-doped phosphors by the reaction of $LaFCO_3$:Ce^{3+} with Al_2O_3 and their luminescence properties

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영남대학교 화학공학부

Ce^{3+}-doped ultraviolet and blue emitting phosphors were prepared by calcining a mixture of $LaFCO_3$:$Ce^{3+}$and Al_2O_3. The emission intensity of the phosphors depended on calcination temperature and F^- concentration. The luminescence spectra of phosphors obtained in an inert gas were similar to that in a reducing gas. The Ce^{3+}-activated phosphors exhibited two emission bands peaking at 352 and 418 nm, which was attributed to $LaAlO_3$:Ce^{3+} and $LaOF$:Ce^{3+}, respectively.

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Enhanced thermoelectric properties of Ba, In, Yb multiple-filled $CoSb_3$ based skutterudites nanocomposites

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With serious concerns on energy conservation and environmental protection, researches for alternative energy sources other than fossil fuels and various energy conversion technologies have been extensively conducted in recent years. Thermoelectric energy conversion, which have been utilized for power generation and solid-state cooling for several decades, is one of the energy conversion technologies that have received much attention for renewable energy production from waste energy or low-grade energy sources. The energy conversion efficiency of thermoelectric devices depends partly on the non-dimensional figure of merit (ZT) of thermoelectric materials. Numerous works have been done to improve the ZT values of thermoelectric materials. For thermoelectric nanocomposites, improvement of ZT values has been suggested due to decrease in lattice thermal conductivity without adverse effects on electrical resistivity. Among many kinds of materials, filled skutterudites are one of the most promising thermoelectric materials for power generation applications, but has a low figure of merit due to the high thermal conductivity. To solve this problem, filling voids with rare earth atoms is an effective way to lowering thermal conductivity which causes scattering of phonons, necessarily enhances thermoelectric properties of skutterudite compounds. In this study, multiple-filled $CoSb_3$ based skutterudite nanocomposites were synthesized by a combination of melting and high-temperature annealing. The structure and composition of the samples are characterized by using XRD, EDS. Thermoelectric characteristics of the filled-skutterudite nanocomposites were evaluated at a temperature range from room temperature to 873 K as a function of the atomic fraction of filler atoms.

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Up-conversion properties depending on various RE3+ ion concentrations of nanophosphors

정종원 B.T.Huy 강지훈 GerelkhuuZayakhuu 이용일*

창원대학교 화학과

Nanoparticle materials have been the subject of increased scientific interest, both for fundamental research and for a wide area of application. Recently, the attention of the nonscientists has been focusing more and more on biological applications. The up-conversion nanoparticles (UCNPs) have many good characteristics. The main materials are that they can emit visible or near infrared (NIR) light under NIR irradiation. In addition, these UCNPs show a sharp emission bandwidth, high photostability, tunable emission, long lifetime, and low cytotoxicity. These benefits make the UCNPs can be used as probes for intravital imaging which enables the investigation of physiological processes within the context of a living organism, and provides a more complete picture of disease pathology and development.Er3+, Tm3+and Yb3+doped NaYF4phosphors were prepared bysolvothermal method. The preparation RECl3 solution (RE = Y, Er, Tm and Yb) for various concentration ratio. This rare earth solution (1 mol/L) added 5ml oleic acid (OA) and 15 ml 1-octadecene (ODE). The solution was heated to 160 oC for 30 min and then cooled down to room temperature. Thereafter, 10 ml methanol solution of NH4F (4 mmol) and NaOH (10 mmol) was added dropwise under stirring for 30 min. After methanol evaporated the solution was heated to 300 oC under nitrogen atmosphere and the temperature should be maintained for 1.0 hr, during this procedure the condenser pipe was needed and the stirring speed was about 1,000 rpm. The resulting nanoparticles were precipitated by the addition of ethanol, collected by centrifugation washed with ethanol several times. Their crystalline structures, surface morphologies and phase transitions were investigated according to annealing process by using X-ray diffraction (XRD), scanning electron microscopy (SEM) and photoluminescence (PL).

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Fabrication of Metallic Nanomeshes for Transparent Electrodes

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경희대학교 응용화학과

Anodic aluminum oxide (AAO) in the form of self-ordered nanopore arrays has drawn much attention as templates to create ordered nanomaterials. Here, we fabricated metallic nanomeshes using AAO membranes as deposition templates. The metallic nanomehses could be used as transparent electrodes for solar cells due to its high conductivity and transparency. Optimized design of transparent electrodes could be achieved by tuning the size and distance of nanopores of metallic nanomeshes.

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WO_3-based Heterojunction Photoanodes for Photoelectrochemical Water Splitting

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Tungsten trioxide (WO_3) has been used as n-type semiconductor photoanodes in a water-splitting photoelectrochemical (PEC) cell. Here, we fabricated Bi_2WO_6/WO_3-based photoanodes with different morphologies through hydrothermal method and followed by annealing with $Bi(NO_3)_3$ solution. WO_3 films were fabricated on FTO by hydrothermal method with different kinds of capping agents which changes the shape of particles. Also, Bi_2WO_6 layers were formed by transforming upper layer of WO_3 films with Bi-solution based annealing. The heterojunction photoanodes showed enhancement in light absorption and PEC performance compared to the plain WO_3 photoanodes. Furthermore, heterojunction films exhibited long-term stability in acidic electrolyte against photocorrosion.

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Biodegradation of electrospun silk fibroin nanofibrous mat by condition of crystallization

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한국기초과학지원연구원 부산센터

The biodegradability, is one of the important parameters for the biomaterials applications, of biopolymer was required for diverse purposes. Therefore, control the biodegradability of biopolymer was an active field of research. In previously study, we reported that it could be control the in vitro and in vivo biodegradability of silk fibroin (SF) nanofibrous mat by treated with various ratio of ethanol/propanol mixtures. In this study, we observed the effect of the ethanol/propanol mixtures on various properties of electrospun SF nanofibrous mat by using FE-SEM, Contact Angle Analyzer, FT-IR, TGA and NMR. As a result, we could suggest that the treatment of various ratio of ethanol/propanol mixture brought the difference conformational transition of SF, which allowed controlling biodegradability of electrospun SF nanofibrous mat

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Copper Selenide as Superionic Conductor with Liquid-like Behaviour and their Thermoelectric Properties

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Thermoelectric materials are used to directly convert heat into electricity. Advanced thermoelectric technology offers a potential for an emission-free method for solid state cooling. Due to the limitation of the high efficiency thermoelectric materials, several theories have been proposed to improve the efficiency of thermoelectric materials. The idea of using the liquid-like behaviour of superionic conductors must be considered an extension of the phonon-glass electron-crystal concept and such materials could be considered phonon-liquid electron-crystal (PLEC) thermoelectrics. Copper chalcogines Cu2-xX (X = S, Se or Te) as the liquid-like behaviour of superionic conductors prepared from chemical synthesis are consolidated to nanostructured bulk pellet using spark plasma sintering (SPS) compaction. Especially, β-phase Cu2-xSe possesses a natural superlattice-like structure that the selenium (Se) atoms form a rigid face-centred cubic lattice and the copper (Cu) layers are disordered around the selenium sublattice. The Se atoms provide a crystalline pathway for semiconducting electrons and the copper ions are superionic with liquid-like mobility, resulting in a low lattice thermal conductivity κL which enables ZT improvement. The results indicate that competing with other conventional commercial materials β-phase Cu2-xSe could be potentially a new direction and interesting for high-efficiency thermoelectric material.

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Improving Solar Cell Efficiency in CdSe Quantum dot/Polymer Hybrid structureby Controllable in Situ polymerization of Thiophene

PHAMQUOCTHAI 이용일* **B.T.Huy**

창원대학교 화학과

Bulk heterojunction solar cell based on CdSe quantum dot (QD)/polythiophene hybrid structure was investigated. Power conversion efficiency of CdSe QD/polythiophene was increased significantly by enhancing the electric interaction between donor and acceptor components. Oleic acid ligands of CdSe QD were exchanged with thiophene monomers, followed by in situ polymerization of the thiophene monomer on the CdSe QD surface. When the polymer was grown on the surface of CdSe QD, the gap distance between quantum dot and conjugate polymer is shorter as compared with that of QD/polymer blend. Thus, increasing the interaction between the two materials and creating a large number of interface for charge transferresult in a shorter PL lifetime, quenched PL intensity, and increased charge transfer rates. This method can facilitate the efficient preparation of the quantum dot/polymer hybrid solar cell with higher power conversion efficiency.

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Catalytic Activity of Magnetically Recoverable Ruthenium Nanoparticles for Organic Reactions

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창원대학교 화학과

Catalysis is becoming a strategic field of science because it represents a new way to meet the challenges of energy and sustainability. The present work explores a facile one pot synthesis of magnetic ruthenium (Fe3O4@Ru) nanocatalysts by chemical co-precipitation method. The synthesized magnetic Ru nanocatalysts are characterized by scanning electron microscopy (SEM), transmission electron microscopy (TEM), X-ray powder diffraction (XRD), thermogavimetric analysis (TGA), X-ray photoelectron spectroscopy (XPS) and vibrating sample magnetometry (VSM). The percentage of Ru in Fe3O4@Ru nanocatalysts is obtained by inductively coupled plasma atomic emission spectroscopy (ICP-AES). As-synthesized Fe3O4@Ru nanocatalysts are applied for suziki coupling, hydrogenation, Himaya cross-coupling and click reactions. The results indicate that the supported Ru catalysts can be conveniently recovered by applying an external magnetic field and the activity of the supported Ru catalyst for organic reactions can still reach up to over 90% after being reused at least five times.

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Controlling the morphology of silver nanowire in the polyol method for the improved transparent conducting electrodes

<u>이호준</u>

부경대학교 화학과

Silver nanowire (AgNW) film meet the requirements of transparent conducting electrodes for many applications and could be an immediate ITO replacement for touch panel electrodes. AgNW have been synthesized by the polyol method in ethylene glycol as a reductant and poly-vinylpyrrolidone (PVP) as a template for growing to one-dimensional formation. In order to fabricate high quality AgNW transparent conducting films, the morphology of AgNW that has thin diameter (10 ㎛) is critical. We studied the critical factors for AgNW morphology by controlling of molecular weight of PVP, relative amount of Ag precursor and other additives in the polyol method. We also prepared AgNW transparent conducting films on flexible substrates such as PET with the synthesized AgNW and a polymer binder and studied the conductivity and transparency of the film. The products were characterized by transmission electron microscopy (TEM) and field emission scanning electron microscope (FE-SEM).

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Multicomponent Cobalt Oxide-Graphene Nanocomposites with Promising Electrode Performance for Lithium Ion Batteries

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이화여자대학교 chemistry [1]이화여자대학교 화학·나노과학과

Multicomponent CoO-layered CoO2-graphene nanocomposites are successfully synthesized by an electrostatically-derived assembly between negatively-charged layered CoO2 nanosheets and positively-modified reduced graphene oxide (rG-O+) nanosheets, which is followed by heat-treatment under reductive atmosphere. The phase composition of cobalt oxide component in the resulting nanocomposites can be tailored by changing heating temperature. The hybridization between cobalt oxide and graphene nanosheets is well-evidenced by electron microscopy and X-ray diffraction analysis. N2 adsorption?desorption isotherm measurements reveal the expanded surface area and mesoporous structure of the resulting nanocomposites, which are attributable to the house-of-cards-type porous stacking of graphene/CoO2 nanosheets. The present nanocomposites exhibit promising anode performance with large capacity and good cycling retention. Of prime importance is that these nanocomposites show excellent rate capability caused by the incorporation of graphene nanosheets. The present phase transformation route using exfoliated metal oxide nanosheet provides a useful methodology to explore novel metal oxide-graphene nanocomposites with promising electrode performance.

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Enhancement of upconversion emission in NaLuGdF4:Yb,Er nanoparticles by co-doping Cr3+

GerelkhuuZayakhuu B.T.Huy 정종원 이용일*

창원대학교 화학과

Upconversion (UC) is a unique type of photoluminescence in which lower-energy excitation (near-infrared light) is converted into higher-energy emission (visible light) via multi-photon absorption processes. The visible green, blue and red upconversion emissions in Yb3+/Er3+ doped NaLuGdF4 nanoparticles were enhanced by co-doping with Cr3+ ions. A possible cause for this could be associated with ionic radius of metal ions doped in host material. The Cr3+ (0.62?) ions were smaller than Lu3+ (0.86?) ions in the host material. The characterization of NaLuGdF4:Yb,Er,Cr3+ were performed by photoluminescence (PL), scanning electron microscope (SEM), X-ray diffraction (XRD) and energy-dispersive X-ray analysis (EDS). The results demonstrate a successful incorporation of Cr3+ ions in NaLuGdF4 :Yb,Er nanoparticles. The effect of Cr3+ on the upconversion luminescence of NaLuGdF4 :Yb,Er was investigated in detail. A possible mechanism for the enhanced upconversion emission is proposed. In addition, these high quality upconversion nanopartilces have a potential for the application in the field of optical nanodevices and biomedicine. Keywords: NaLuGdF4 :Yb,Er, upconversion nanoparticles, co-doping chromium ions

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Synthesis of a New CdSe$_{1\text{-}x\text{-}y}$S$_x$Te$_y$ nanocrystals

최인녕 B.T.Huy 이용일*

창원대학교 화학과

Recently, nanocrystals were developed for improving the efficienby of solar cells. A new CdSe1-x-ySxTey nanocrystals were synthesized using thioglycolic acid as a stabilizing agent in aqueous system.The composition of the CdSe1-x-ySxTey nanocrystals was controlled by tunning the ration of Se/S/Te . The optical properties of the nonocrystals waer investigated depending on the ratios of Se, S and Te. The structural, morphological, and optical properties of the nanocrystals were analyzed using X-ray diffraction (XRD), field emission transmission electron microscope (FE-TEM), energy dispersive X-ray spectroscopy (EDS), and photoluminescence (PL) measurements. The results show that CdSe1-x-ySxTey nanocrystals are a promising material for solar cell application.

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Enhanced Photoelectrochemical Performance of Silicon Nanowire Photocathodes Decorated with MoS_2 Nanoparticles

이정은 이민형*

경희대학교 응용화학과

P-type silicon has been widely used as photocathodes for solar assisted water splitting cells because of high visible absorption and earth abundance. Although photocurrent of Si cathodes currently reach to theoretical maximum level with nanotexturing such as Si nanowire (SiNW), photovoltage of SiNWs is still not enough to provide half of required potential for water splitting. Here, we fabricated SiNW photocathodes decorated with several types of MoS_2/rGO catalysts to improve photovoltage. Morphology of MoS_2 nanoparticles on rGO were controlled by changing graphene component. PEC performance of SiNW photocathodes were depending on surface area of catalytically active edge site of MoS_2. Also, long-term stability of SiNW photocathodes were also improved by passivation effect of rGO.

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Dye-sensitized solar cells with p-doped three-dimensional graphene counter electrode

안효진 김선이[1] 장지현[1,*]

울산과학기술대학교(UNIST) 친환경에너지공학부 [1]울산과학기술대학교(UNIST) 친환경 에너지 공학부

We fabricated p-doped 3D graphene networks (3D-GNs) as counter electrode materials for dye-sensitized solar cells (DSSCs), which show the superior catalytic property to platinum counter electrode. The 3D-GNs with the high surface area and conductivity are prepared via a CVD growth process and then a mild doping process is conducted to improve the conductivity and catalytic property by adding oxygen and nitrogen molecules onto the surface of the 3D-GNs. The oxygen and nitrogen contents of the 3D-GNs are optimized by varying treatment time of HNO3. An optimized 3D-GN based DSSC exhibits a 6.01% higher photoconversion efficiency (8.46%) than a pt based DSSC due to enhanced conductivity and catalytic activity.

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Mechanistic Understanding of the Phase Transition and Characteristic Features Change from $GdPO_4:Eu^{3+}$?H_2O Nanorods to $GdPO_4:Eu^{3+}$ Nanoparticles

<u>조준상</u> 김창해[1,*]

한국화학연구원 화학소재본부/박막재료연구그룹 [1]한국화학연구원 화학소재연구단

$GdPO_4:Eu^{3+}$?H_2O nanorods were synthesized by simple co-precipitation route and transformed to $GdPO_4:Eu^{3+}$ nanoparticles after annealing at 900 ?C. It indicated that as-prepared $GdPO_4:Eu^{3+}$?H_2O nanorods with hexagonal phase were transformed to $GdPO_4:Eu^{3+}$ nanoparticles with monoclinic phase around 800 ?C due to the release of water molecules incorporated in hexagonal crystal lattice. Niroj et al reported that the evaporation of water molecules in hexagonal axis was key to induce phase transition but the phase transition mechanism has not investigated in-depth. Thus, in our report, we demonstrate a general strategy for the synthesis of high crystalline $GdPO_4:Eu^{3+}$ nanorods and nanoparticles, and systematically study the phase transformation and relevant multifunction changes from $GdPO_4$?$H_2O:Eu^{3+}$ nanorods to $GdPO_4:Eu^{3+}$ nanoparticles. During phase transition, the in situ measurements TEM and XRD are carried out so that we can understand the phase transformation mechanism via heat treatment as well as investigate corresponding properties change in order to design, develop, and optimize the multifunctional contrast agent with highly efficient in luminescent and magnetic properties. Ultimately, the $GdPO_4:Eu^{3+}$ nanoparticles have both excellent luminescent properties of strong red emission at 592 and 610 nm and MR properties can be potentially used as efficient multifunctional nanoprobes for bio-imaging.

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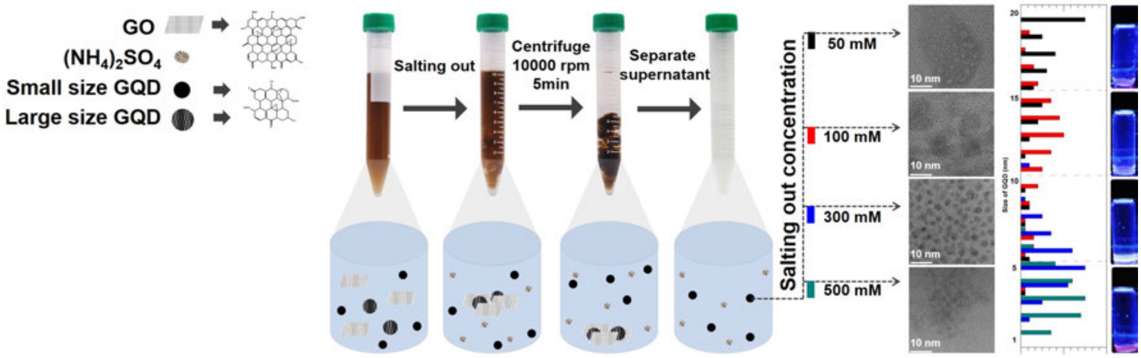
Quantum Size Effects on Photoluminescence in Graphene Quantum Dots

이규의 이해신*

한국과학기술원(KAIST) 화학과

In this study, we report a method that can effectively sort GQDs with various dimensions. The method simply utilizes the addition of salts to a heterogeneous mixture of GQD solutions. The purification process is based on differences in dispersibility of individual GQDs as a function of salt concentrations. We found that a salt can distinguish tiny differences in physical properties of GQDs, resulting in the separation of GQDs with narrow windows of physicochemical properties of GQDs. Well-purified GQD subpopulations exhibited GQDs with average diameters of 2.7 ± 1.4 nm, 5.1 ± 1.9 nm, 13.3 ± 3.11 nm, and 18.7 ± 4.44 nm. Consequently, each of GQD subpopulations exhibited blue purple, blue, yellow green and orange emission properties in 325nm excitation condition. These results demonstrate that salts are effective additives in purifying size dependent GQD subpopulations which is entirely new way of spectral tuning.



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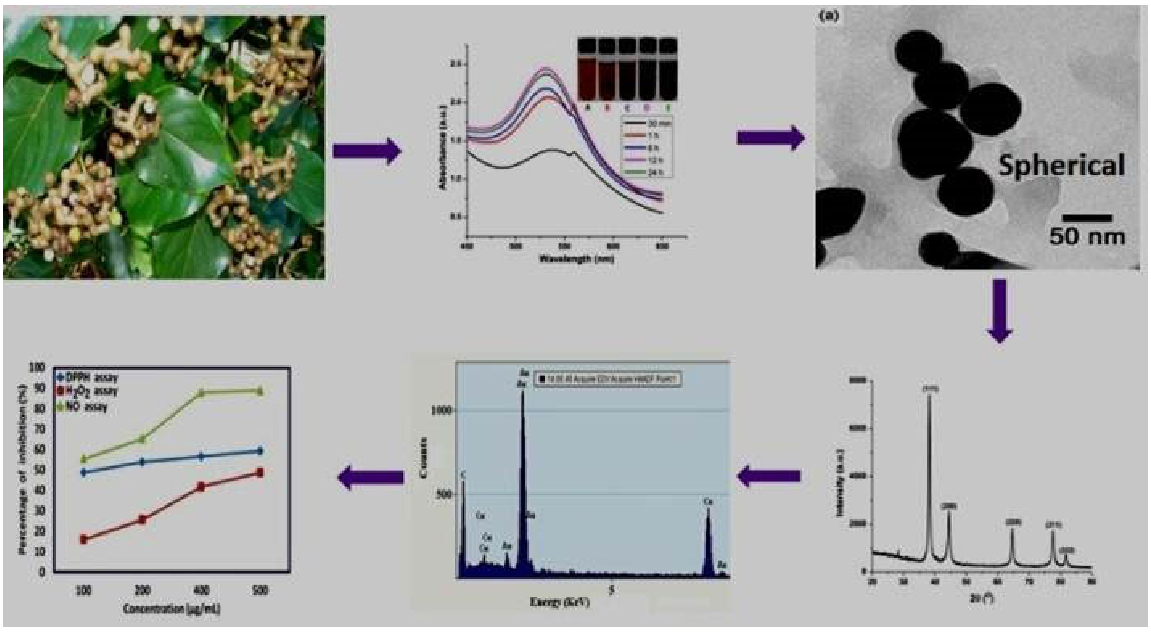
Biosynthesis of Gold Nanoparticles Using Hovenia dulcis Fruit Extract and Their Biomedical Potentials

POUDELTEJNARAYAN BASAVEGOWDANAGARAJ 이용록*

영남대학교 화학공학부

We describe the synthesis of gold nanoparticles (GNPs) at room temperature using an aqueous extract of Hovenia dulcis fruit and the antioxidant and antibacterial activities of the GNPs obtained. The devised method provides a simple, cost-effective aqueous means of producing spherical and hexagonal GNPs of size ～20 nm. The synthesized GNPs were characterized by UV-visible spectrum and obtain a peak at 536 nm. Fourier transform infrared (FT-IR) spectroscopy results showed that the extract containing some biomolecules accountable for both reducing as well as capping gold ions into GNPs. Transmission electron microscopic (TEM) studies of the particles revealed a dominance of spherical particles with a very few hexagonal GNPs. The face centered cubic structure of the GNPs was con?rmed by X-ray diffraction (XRD) peaks at 38º, 44º, 64º and 77º, which were indexed to the (1 1 1), (2 0 0), (2 2 0), and (3 1 1) planes with clear circular spots in the selected area electron diffraction (SAED). Elemental analysis was performed by energy dispersive X-ray analysis (EDX). In addition, the authors investigated in vitro antioxidant and antibacterial properties of the biosynthesized GNPs, which were found to be significant.


Absorbance (a.u.)
Wavelength (nm)
30 min
1 h
6 h
12 h
24 h
A
B
C
D
E
(a)
Spherical
50 nm
Intensity (a.u.)
2θ (°)
(111)
(200)
(220)
(311)
(222)
Counts
Energy (KeV)
C
Cu
Au
DPPH assay
H2O2 assay
NO assay
Percentage of inhibition (%)
Concentration (µg/mL)

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Controlled Growth of In-plane Heterostructure of Graphene and Hexagonal Boron Nitride on Platinum

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The lateral heterostructure of hybridized graphene and hexagonal boron nitride (h-BN) has attracted particular attention in research of two dimensional (2D) materials. However, the control of the interface formation in the heterostructure is one of great challenges in 2D materials. Recently, patterned regrowth method has been attempted for the controlled synthesis of lateral junctions between graphene and h-BN. However, many fundamental understandings are still not clear, including the in-plane atomic continuity as well as the edge structure of graphene.

In this presentation, we report lateral heterostructures of hybridized graphene and h-BN by the chemical vapor deposition (CVD) method. The lateral heterostructures were grown by using Pt foil as the substrate and ammonia borane and methane gas as precursors. The heterostruture grown on Pt foil could be successfully transferred onto an arbitrary substrate via an electrochemical bubbling-based method. Thus, the interface formation of the heterostructures was investigated by Raman spectroscopy, scanning tunneling microscopy, and high-resolution transmission electron microscopy (HR-TEM).

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Effect of Pressure on Growth of MoS_2 by Low-Pressure Chemical Vapor Deposition

안성준 신현석[1,*]

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Transition Metal Dichalcogenides (TMDs) as layered structures like graphene shows outstanding mechanical, optical, and electrical properties in single layer or few layers that is chemically stable . For example, the band gap energy of single-layer MoS_2 is 1.8 eV which is larger than that of bulk MoS_2, 1.2 eV. This value, 1.8 eV, is an ideal band gap for the channel material of a logic transistor which can have the mobility of at least 200 $cm^2 V^{?1} s^{?1}$, similar to that of graphene nanoribbons. [1] More interesting thing is mechanical measurements performed on single-layer MoS2 show that it is a flexible and strong material with a high Young's modulus, comparable to stainless steel. [2]

In this presentation, we report growth of MoS_2 on various substrates which is controlled by pressure in a tube of a chemical vapor deposition (CVD) system. The MoS_2 layers were grown using MoO_3 and sulfur powders as precursors in the low-pressure CVD system. The precursors are decomposed to atomic species which recombines on the surface of the substrate. Thus, the growth of MoS_2 is affected by pressure of the CVD system.

Reference

[1] B. Radisavljevic, A. Radenovic, J. Brivio, V. Giacometti and A. Kis, Nat. Nanotechnol. 6(3), p.147 (2013).

[2] S. Bertolazzi, J. Brivio, A.Kis, ACS nano 5(12), p.9703 (2011).

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Hydrogenation of Grapahene: Formation of Diamond-Like Film

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Diamond possesses a number of exceptional properties such as the highest hardness, the lowest thermal expansion coefficient, and high thermal conductivity at room temperature. Transforming graphite to diamond is needed to apply high temperature and high pressure. As an alternative way to obtain diamond, theoretical studies suggest that multilayers of graphene can be transformed to sp^3 hybridized diamond-like structure by hydrogenation or fluorination at room temperature.[1]

In this presentation, we report hydrogenated graphene multilayers *via* the simple hydrogen plasma treatment. Graphene was grown on Cu foil by low-pressure chemical vapor deposition (CVD) system. 2-layers, 3-layers, and 4-layers of graphene were prepared by the wet transfer method with single-layer graphene on Cu foil. We confirmed that the graphene multilayers remained without any damage after hydrogen plasma treatment by scanning electron microscope (SEM). Further, we characterized the hydrogenated graphene multilayers by using Raman spectroscopy, UV/Vis spectroscopy, XPS, and 4-point probe measurement.

Reference

1. Rajasekaran, S.; Abild-Pedersen, F.; Ogasawara, H.; Nilsson, A.; Kaya, S Phys. Rev. Lett. 111, p.085503. (2013)

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One-pot mass production of polymer microspheres embedding CNT-taxol complexes using an ammonium-based room temperature ionic liquid for controlled drug delivery

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단국대학교 나노바이오의과학과 [1]단국대학교 나노바이오의과학

We describe herein a new methord for one-pot mass production of microspheres of polymer and polymer-CNT-drug using an ammonium-based room temperature ionic liquid. Polycaprolactone (PCL), trioctylmethylammonium chloride (TOMAC; liquid state = -20 ~ 240 ^{o}C), and taxol were used as a model substrate, respectively, for polymer, room temperature ionic liquid, and drug. A large quantity of white colored PCL powder and gray colored PCL-CNT-taxol powder were produced via a phase separation between the hydrophilic ionic liquid and the hydrophobic substrates from their mixture solution. The particles showed uniform and spherical structure of average 15 um in diameter. Taxol embedded in the PCL-CNT-taxol microbeads was proven by ^{1}H-NMR analysis to be about 1 ug per 0.1 mg polymer and consistant taxol-releasing was confirmed to be 0.18 ug per 7 days by HPLC.This symple method to fabricate microspheres may be potentially useful as an one-pot method to prepare drug-loaded microspheres.

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Bucky-sponge consisting of MWCNTs functionalized with chitosan: Porosity control using room temperature ionic liquids (RTILs)

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단국대학교 나노바이오의과학과 [1]단국대학교 나노바이오의과학

Here we present CNT bucky-sponges with different porosities and cross-linked with chitosan skin. The nano- and micro-porous and three dimensionally interconnected carbon-structure was created by using an imidazolium based room temperature ionic liquid (RTIL). The nano- and micro-pores with various aspect ratio (about ^{2}/g and about 5 to 28 %. The prepared CNT sponges showed all the important characteristics indicating broad applicability as conductive polymer framework, drug carrying scaffold, catalyst supports, oil adsorbents, and molecular sieve membranes.

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Graphene Oxide/Peptide-Quencher Hybrids for Optical Detection of Cell-Secreted Proteases by Turn-on Response

양진경 이윤식*

서울대학교 화학생물공학부

Proteases are of great relevance to physiological and pathological processes, and thus, have been used as biomarkers in the fields of biology, medicine and biotechnology. There have been continuous interests to develop a simple, rapid and sensitive sensing tool for monitoring protease activity over the past decades. Detection strategy using fluorescence resonance energy transfer (FRET) between substrate-dye and quencher has emerged as alternative. In particular, graphene oxide (GO) based sensing platform have attracted great attentions due to the properties of GO, such as biocompatibility, chemical affinity to biomolecules, and fluorescence quenching ability. Here, we construct GO-peptide-quencher to utilize inherent fluorescence of GO for optical detection of protease activity. Then, we have examined quenching efficiency of various quencher molecules such as metallo protoporphyrin derivatives (MePPs) and QXL_{570} and present their quenching mechanism. This sensing system detects protease activity by recovery of GO fluorescence and successfully monitors cell-secreted MMP-2 in living cells, human hepatocytes HepG2.

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Fabrication of TiO_2 Hollow Spheres / TiO_2 Nanoparticles Photoanode : Improved Performance in Dye-Sensitized Solar Cells

박수경 배재영[*]

계명대학교 화학과

The TiO_2 hollow spheres are synthesized by a core-shell method. Compared to conventional P25 TiO_2 nanocrystalline particles, the TiO_2 hollow structured materials not only have a low density, high specific surface areas, and hierarchically porous structures but also exhibit high light-scattering efficiency and fast motion of the charge carriers. The photoelectrode consisting of TiO_2 hollow spheres and TiO_2 nanoparticles for use in dye-sensitized solar cells (DSSCs) is prepared, the performance of DSSCs are investigated. Improved performance of the DSSCs is obtained compared with the P25 TiO_2 nanocrystalline DSSCs. The improved performance is mainly due to the enhanced light scattering by the TiO_2 hollow spheres. The open circuit voltage of the hollow spheres modified DSSCs is higher than that of the DSSC with pure P25 photoanode, which can be attributed to the fact that TiO_2 hollow spheres substitute of the TiO_2 nanocrystallines and reduce the interface recombination by decreasing the surface charge trap-site density of the photoanodes.

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Preparation and Characterization of Hollow Silica Spheres with Mesoporous Shell by Sol-gel method

진현탁 배재영*

계명대학교 화학과

Synthesis of hollow mesoporous silica spheres (HMSS) through directed surface sol-gel process of tetraethylorthosilicate (TEOS) on the template of core-shell microspheres of polystyrene in the presence of the CTACl surfactant is discussed. Transmission electron microscopy (TEM), X-ray diffraction (XRD) and Brunauer- Emmett-Teller method (BET) analysis are applied to characterize the synthesized HMSS. Well defined HMSS with shell thickness ranging from 12 to 18 nm were synthesized. The result materials XRD showed mesoporous structered and BET surface area was 941 m^2/g.

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Preparation of Vinyl Functionalized Mesoporous Milica by Hydrogen Gas Adsorption

구병진 배재영*

계명대학교 화학과

Vinyl functional groups with mesoporous silica was prepared by sol-gel method. This method is using tri-block copolymer surfactant and CTACl as a template. Preparation of mesoporous silica was by adjusting the molar ratio of the silica and surfactant. The preparation of vinyl functionalized mesoporous silica was characterized by Brunauer-Emmett-Teller (BET) method, Transmission electron microscopy (TEM), FT-IR and Temperature programmed reaction (TPR).

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발표코드: **MAT.P-1077**

발표분야: 재료화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

Synthesis and Characterization of Hexagonal and Cubic Structrued Mesoporous Silica with High Surface Area

서원호 배재영*

계명대학교 화학과

A solution based processing method has been used to synthesized mesoporous silica materials using tetraethylorthosilicate (TEOS) and cetyltriammonium chloride (CTACl). The result materials were characterized by transmission electron microscopy (TEM), X-ray diffraction (XRD), and BET surface area. The diameters of mesoporous is afford to controlled in range from 300 to 350 nm. mesoporous silica materials XRD showed hexagonal and cubic structured. BET surface area was 1139 m^2/g high surface area.

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

Preparation of TiO_2 sol solution which is controlled a particle size by concentration and reaction time

김재욱 배재영*

계명대학교 화학과

Titanium dioxide (TiO_2) sol solutions, which was prepared by sol-gel hydrothermal method using Titanium tetraisopropoxide as a precursor. TiO_2 sol was prepared by H_2O and HCl. During the stirring, TiO_2 sol is sampled every 2 hours. The resulting materials were characterized by particle size distribution, transmission electron microscopy (TEM) and X-ray diffraction (XRD). Particle size distribution results showed 8 nm ~ 200 nm size of particle in sol solution.

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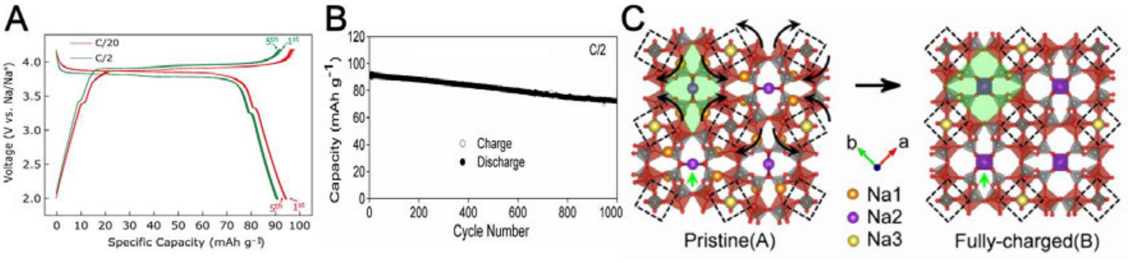
발표종류: 포스터, 발표일시: 수 16:00~19:00

Role of intermediate phase for stable cycling of $Na_7V_4(P_2O_7)_4PO_4$ in sodium ion battery

임수연 최장욱[1,*]

한국과학기술원(KAIST) EEWS 대학원 [1]한국과학기술원(KAIST) EEWS

Utilizing low-cost materials, sodium ion batteries (SIBs) are beginning to attract considerable attention, particularly for large-scale utility grid applications. However, electrochemical performance of most SIB active materials is still insufficient for various practical applications. In this talk, I will present a vanadium-based ortho-diphosphate, $Na_7V_4(P_2O_7)_4PO_4$, that holds exceptional electrochemical properties such as well-defined high voltage profiles at 3.88 V (vs. Na/Na+) and substantial capacity retention over 1,000 cycles. Furthermore, a combined theoretical and experimental investigation revealed that single-value voltage behavior and long cycle life originate from iso-energetic structural rearrangement in the presence of an intermediate phase. Based on this interpretation, we propose that the presence of intermediate phases would support better kinetics during phase transformation and is a general guidelines in future electrode design in SIBs.



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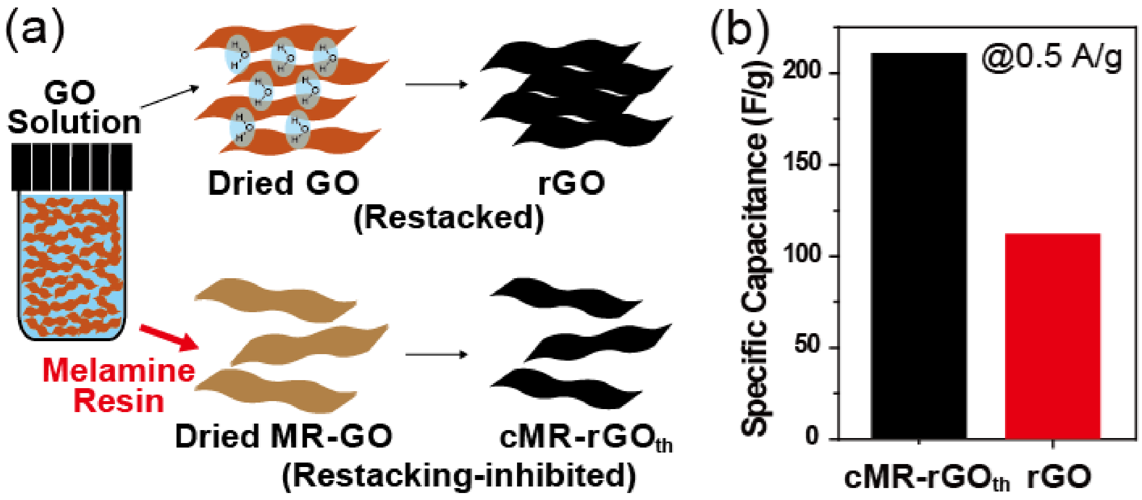
발표코드: **MAT.P-1080**
발표분야: 재료화학
발표종류: 포스터, 발표일시: 수 16:00~19:00

Restacking-Inhibited 3D Reduced Graphene Oxide for High Performance Supercapacitor Electrodes

이지훈 최장욱*

한국과학기술원(KAIST) EEWS

Graphene has received considerable attention in both scientific and technological areas due to its extraordinary material properties originating from the atomically single- or small number-layered structure. Nevertheless, in most scalable solution-based syntheses, graphene suffers from severe restacking between individual sheets and thus loses its material identity and advantages. In the present study, we have noticed the intercalated water molecules in the dried graphene oxide (GO) as a critical mediator to such restacking and thus eliminated the hydrogen bonding involving the intercalated water by treating GO with melamine resin (MR) monomers. Upon addition of MR monomers, porous restacking-inhibited GO sheets precipitated, leading to the carbonaceous composite with an exceptionally large surface area of 1040 m2/g after a thermal treatment. Utilizing such high surface area, the final graphene composite exhibited excellent electrochemical performance as a supercapacitor electrode material: specific capacitance of 210 F/g, almost no capacitance loss for 20000 cycles, and ~7 sec rate capability. The current study delivers a message that various condensation reactions engaging GO sheets can be a general synthetic approach for restacking-inhibited graphene in scalable solution processes.


(a)
GO
Solution
Dried GO
rGO
(Restacked)
Melamine
Resin
Dried MR-GO
cMR-rGO$_{th}$
(Restacking-inhibited)
(b)
@0.5 A/g
Specific Capacitance (F/g)
0
50
100
150
200
cMR-rGO$_{th}$
rGO

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

Urea pyrolysis route to Zn-rich $(GaN)_{1-x}(ZnO)_x$ solid solution from Zn_2Ga layered double hydroxide

양재훈 PEIYIRONG 최진호*

이화여자대학교 화학.나노과학과

$(GaN)_{1-x}(ZnO)_x$ solid solution is one of the promising visible-light harvesting photocatalysts for overall water-splitting. We could find the novel synthetic route to $(GaN)_{1-x}(ZnO)_x$ solid solution by two-step pyrolysis of urea with Zn_2Ga layered double hydroxide (LDH) at different temperature. We first calcined the mixture of urea and Zn_2Ga -LDH with the molar ratio of Urea/Ga = 12 at 673 K under N_2 flow, resulting in the amorphous material. We could synthesize $(GaN)_{1-x}(ZnO)_x$ solid solution with yellow color via pelletizing and calcining the amorphous material at 1123 K under nitrogen flow. According to XRD analysis, $(GaN)_{1-x}(ZnO)_x$ solid solution was successfully prepared without any impurity. By using urea instead of ammonia, the reaction time was shortened to 2 hours, and the absorption edge of thus prepared $(GaN)_{1-x}(ZnO)_x$ was red-shifted compared to that of the solid solution prepared from ZnO and Ga_2O_3 under ammonia gas flow. The bandgap energy and Zn content of the solid solution were determined to be 2.42 eV and x = 0.52, respectively, which is smaller bandgap energy and much higher Zn content than $(GaN)_{1-x}(ZnO)_x$ prepared via ammonia nitridation method (2.72 eV, x = 0.15). This urea pyrolysis method could be applied to synthesizing various metal oxynitrides and controlling their bandgap.

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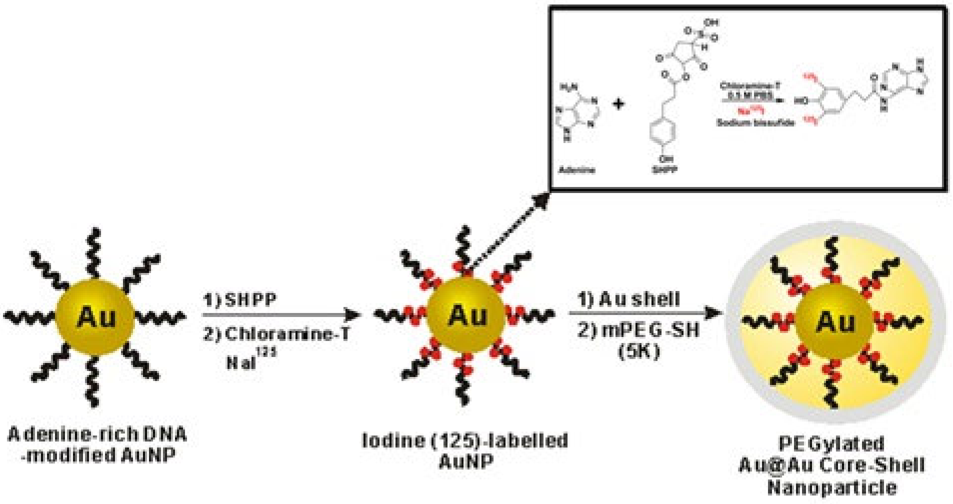
발표종류: 포스터, 발표일시: 수 16:00~19:00

DNA-Modified Au Core and Au Shell Nanoparticle for Highly Sensitive and Stable SPECT Imaging Probe

이상봉 **KumarDinesh**[1] 김수민 국현[2] 임동권*

전북대학교 BIN 융합공학과 [1]Chonbuk National Uni BIN Fusion Tech. [2]전북대학교 BIN융합공학과

Abstract: The radio-isotope labelled biomolecules (i.e., peptide, protein) have been widely used as in-vivo imaging probe, but suffer from fast excretion, off-target effect, and lack of biological stability. It has been known that the use of nanoparticle can alter the pharmacokinetics and pharmacodynamics of conventional drug molecules. In this regards, nano-sized imaging probe with high sensitivity and excellent biological stability was greatly demanded. Here, we report highly sensitive and stable SPECT imaging probe by use of simple chemistry of sodium iodide (125) and adenine-rich oligonucleotide modified AuNP, and seed-mediated Au shell growth in solution. In theory, two thousands of Iodine-125 can be covalently conjugated to DNA base per gold nanoparticle (20 nm), which can greatly increase the radio sensitivity of nanoparticle. Iodine-125 embedded Au@Au nanostructure was synthesized by forming uniform Au shell with 10 nm thickness, which can improve the stability of Iodine-125 label on gold nanoparticle by preventing possible hydrolysis or enzymatic attacks in in-vivo. Three different diameter of Iodine-125 embedded Au@Au nanostructure (27, 32, 42 nm) were prepared to investigate radio sensitivity, biological stability, and in-vivo distributions for efficient SPECT imaging. A series of analysis showed highly sensitive radio activity, increased stability of Au@Au nanostructure, and size-dependent particle distributions in normal mice.


H2N
Adenine
+
OH
SHPP
Chloramine-T
0.5 M PBS
Na125I
Sodium bissufide
125I
HO
125I
Au
Adenine-rich DNA -modified AuNP
1) SHPP
2) Chloramine-T NaI125
Iodine (125)-labelled AuNP
1) Au shell
2) mPEG-SH (5K)
PEGylated Au@Au Core-Shell Nanoparticle

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발표분야: 전기화학

발표종류: 포스터, 발표일시: 수 16:00~19:00

[발표취소] Cathode Performance of Layer-Structured $LiMnO_2$ and Polypyrrole Composites for Li Ion Batteries

김아연* 여인형[1] 모선일

아주대학교 에너지시스템학부 화학 [1]동국대학교 화학과

발 표 취 소

본 논문은 발표취소된 논문입니다.

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발표종류: 포스터, 발표일시: 수 16:00~19:00

[발표취소] Preparation and Characterization of Nanocryatalline Li_2MSiO_4(M=Mn,Fe) Cathodes

김아연* 여인형[1] 모선일

아주대학교 에너지시스템학부 화학 [1]동국대학교 화학과

발 표 취 소

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Effect of pH on the Anodic Formation of Nanoporous Gold Films in Chloride Solutions: Optimization of Anodization toward Ultrahigh Porous Structures

김민주 김종원*

충북대학교 화학과

나노다공성 금속 구조체는 균일한 표면 구조를 지니며, 매우 큰 표면적을 가진다. 이에 따라 높은 촉매적 활성을 보이며, 전기화학적으로 안정한 구조를 가지게 되어 많은 연구에 응용 가능성을 보여주고 있다. 이를 형성하는 다양한 방법 중에서도 양극산화 반응은 상대적으로 간단하게 나노다공성 구조체를 형성할 수 있다는 장점이 있다. 본 연구에서는 염소 이온 존재 하에서 양극산화 반응을 이용하여 금 표면에 나노다공성 구조를 형성시켰으며, 가해주는 전위와 용액의 pH 의 영향을 관찰하였다. 그 결과 이 구조는 특정 전위를 가해줄 때만 형성이 됨을 확인하였다. 이는, pH 에 따라 $AuCl_4^-$ 가 생성되는 전위는 변화가 없었지만 금 산화물이 형성되는 전위에는 많은 영향을 받는다는 것과 관련이 있음을 확인하였다. 이를 통해 최적의 전위와 pH 조건을 찾아, 형성 시간을 증가하여 나노다공성 구조를 형성시켰다.이로써, 기존의 선행연구들과 비교하여 보다 효율적으로 짧은 시간 동안 매우 큰 표면적을 얻을 수 있었다. 형성한 구조는 주사 전자 현미경과 X 선 광전자 분광법을 통해 구조적 특성을 확인할 수 있었다. 또한, 최적의 조건으로 형성한 전극으로 글루코오스 전류법 검출을 통해 높은 민감도와 선택성이 나타나는 결과를 얻었다. 이를 통해 나노다공성 금 전극이 글루코오스의 전기화학적 검출에 효과적으로 응용 가능할 것으로 예상한다. [본 연구는 교육부와 한국연구재단의 지역혁신인력양성사업으로 수행된 연구결과임 (No. 2012H1B8A2026112)]

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

Shape-controlled palladium nanostructures: superhydrophobicity and electrocatalytic properties

이금섭 김종원*

충북대학교 화학과

팔라듐은 포름산 산화반응에 있어 촉매 활성이 우수하다. 특히, 팔라듐 나노구조체는 다양한 모양으로 형성되어 순수한 팔라듐보다 더 높은 촉매적 활성을 가지기 때문에 많은 연구가 진행되고 있다. 그러나 그 중요성에 반하여 팔라듐 나노구조체의 모양과 촉매 현상의 연관성에 대한 연구는 아직 미흡하다. 본 연구에서는 전기화학적 석출 방법을 통해 indium tin oxide (ITO) 표면에 K_2PdCl_4 의 농도와 석출 전위를달리하여 세 가지 서로 다른 모양의 팔라듐 나노구조체를 형성하였고, 형성 구조에 따른 전기화학적 촉매 현상을 포름산 산화반응을 이용하여 관찰하고 규명하였다. 또한 대 시간 전류법을 통해서 지속적인 포름산 산화반응에서의 안정성 검사도 진행하였다. 다음으로 나노구조체의 모양에 따른 젖음성의 변화를 접촉각 측정을 통해서 관찰하였다. 주사 전자 현미경을 통해 각각 둥근 구조, 각진 구조, 뾰족한 구조의 형성을 확인하였다. 뾰족한 구조는 포름산 산화 반응에 가장 우수한 촉매적 활성을 보인 반면, 포름산의 지속적인 산화반응에서의 안정성은 둥근 구조에서 가장 뛰어났다. 그리고 접촉각 측정에 있어서는 각진 구조가 155° 로 가장 높은 접촉각을 가지는 결과를 보이며, 이는 초소수성임을 확인하였다. 이러한 결과를 이용하여 형성 구조에 따른 활성을 비교, 평가함으로써 팔라듐 나노구조체의 다양한 응용 가능성을 제시할 수 있다. [본 연구는 교육부와 한국연구재단의 지역혁신인력양성사업으로 수행된 연구결과임 (No. 2012H1B8A2026112)]

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Fabrication of Porous Pt Ball Structure by Simple Electrodeposition and Their Electrochemical Detection of Glucose

노성진 김종원*

충북대학교 화학과

다공성 백금 구조체는 큰 표면적을 가짐과 동시에 백금이라는 금속의 고유한 특성으로 인해 다양한 반응에 있어 촉매적 활성이 뛰어나다. 따라서 다공성 백금 구조체를 형성하기 위한 다양한 방법들이 많이 연구되어 왔다. 백금과 다른 금속의 합금을 형성하는 방법과, 형판을 이용하여 백금 구조를 형성하는 방법, 그리고 환원제를 이용한 화학적 합성 기법이 보고된 바 있다.본 연구는 전기화학적 석출법을 이용하여 형성한 다공성 백금 공이라는 독특한 구조를 주사 전자 현미경 (Scanning Electron Microscopy, SEM) 을 통해 확인하였고 글루코오스의 산화 반응을 관찰하는 연구를 수행하였다. 다공성 백금 공 형성 과정에서 석출 전위의 변화에 따른 구조의 경향을 관찰하였으며, -0.8 V 의 일정한 전위를 가해 주는 경우 일정한 크기를 가진 백금 공이 형성됨을 확인하였다. 또한 석출 전하를 변화시켜 다공성 백금 공 구조의 형성 과정을 관찰하였을 뿐 아니라, 전하의 증가에 따른 다공성 백금 막 구조의 두께 변화를 통해 다양한 두께의 다공성 백금 공 구조 중에서 글루코오스 산화 활성을 가장 극대화할 수 있는 최적 조건은 0.3 C 이었다.형판 또는 환원제를 이용하지 않은 매우 간단한 방법으로 형성시킨 순수한 백금으로 이루어져 있는 다공성 백금 공 구조 상에서 글루코오스의 전류법 검출 결과를 통해 글루코오스 센서뿐만 아니라, 백금 나노 구조로서의 다양한 응용 가능성을 제시하고 있다. [본 연구는 교육부와 한국연구재단의 지역혁신인력양성사업으로 수행된 연구결과임 (No. 2012H1B8A2026112)]

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Ultrasound assisted synthesis of Spinel Manganese-Cobalt Oxide Nanoparticles as Electrocatalyst for Oxygen Reduction Reaction in Alkaline Media

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In this work, we report the sonochemical preparation of spinel manganese-cobalt oxide NPs and their electrochemical properties for oxygen reduction reacton in alkaline media. To the best of our knowledge, this is the first work which is investigation of composition dependent ORR activity on manganese-cobalt oxide materials in keeping the cubic structure. Our metal oxide nanoparticles (MON) with various compositions are denoted as (MON-1, MON-2, MON-3, MON-4, MON-5 and MON-6). Among the manganese-cobalt oxide materials, MON-2 sample shows the higher ORR current and onset potential in 0.1 M KOH aqueous solution. Furthermore, limited current density and electrochemical stability of MON-2 sample are higher than that of Pt/C(premetek). These results show the importance of composition control in the design of highly efficient ORR electrocatalyst.

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$Ni(OH)_2$ dendrite for electrochemical glucose sensor

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A nonenzymatic electrochemical sensor was fabricated for glucose detection based on $Ni(OH)_2$ dendrite. The $Ni(OH)_2$ was electrodeposited on Cu dendrite, which was fabricated by chronoamperometry (CA) at -0.5 V. The thickness of $Ni(OH)_2$ was controlled by deposition time and current. The stem-length of the dendrite was about 30 m and the diameter of branches within each dendrite was about 320 nm. The structure and composition of $Ni(OH)_2$ dendrite were confirmed by scanning electron microscopy (SEM), energy dispersive X-ray analyses (EDX), X-ray diffraction spectrum (XRD), and X-ray photoelectron spectroscopy (XPS) analysis. The mechanism and kinetics of the electro oxidation of glucose were investigated by cyclic voltammetry (CV) and chronoamperometry (CA). The $Ni(OH)_2$ dendrite electrode exhibited high electrocatalytic activity and good response toward the oxidation of glucose in alkaline solution, attributing to the high surface area. At detection potential of + 0.6 V, the biosensor exhibited high sensitivity of 2082 $\mu AmM^{-1}cm^{-2}$ for glucose with a wide linear range from 1 μM to 4.5 mM as well as a low detection limit of 0.24 μM (S/N=3). The good analytical performance, low cost, and simple fabrication procedure make this novel electrode material promising for the development of effective non-enzymatic glucose sensor.

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Fabrication of hierarchical structured MnO_2 by using pulse technique and surfactant for a supercapacitor electrode

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Hierarchical structured MnO_2 was prepared by using pulse technique and surfactant on gold plate. The morphology of MnO_2 was controlled by varying the conditions: applied potential, amount of surfactant, and reaction time. The chemical composition and the crystallinity of MnO_2 were confirmed by X-ray photoelectron spectroscopy (XPS) and X-ray diffraction spectroscopy (XRD), and the morphology of the MnO_2 was investigated by scanning electron microscope (SEM). The micro petal-like MnO_2 structure was observed, and a lot of nano-sized branches were grown on the surface of the petal depended on the reaction time. Electrochemical properties of the MnO_2 electrode were also studied by cyclic voltammetry and impedance spectroscopy. Hierarchical structured MnO_2 provide channels for electrolyte access and fast electron conducting. Therefore, the MnO_2 electrode exhibits high capacitance

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CO Tolerance Performance of Pt-Mesoporouos Metal Oxide Nanocomposite Thin Films for Methanol Oxidation Reaction by Strong Metal-Support Interaction

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We report a highly improved kinetics with superior CO tolerance in an electrocatalytic methanol oxidation reaction (MOR) on platinum-mesoporous metal oxide composite thin films. Pt-mesoporous metal oxide composite films were synthesized by two-step process. First, mesoporous tin oxide thin films (MSnTFs) and mesoporous gallium oxide thin films (MGTFs) with wormlike structure were prepared by sol-gel method. And then, Pt is deposited into the pores of MSnTFs and MGTFs by using electrochemical deposition method. In the results of electrochemical experiments as CO stripping and MOR, these samples showed the meaningful phenomena. Interestingly, we observed the pre-peak of CO stripping at 0.25 V, much lower potential than that of main peak, according to oxidation of weaker adsorbed CO molecules. In addition, these results were related to the explanations of effective enhancement of MOR. The properties of Pt-MSnTFs and Pt-MGTFs were characterized by scanning electron microscopy (SEM), transmission electron microscopy (TEM) and x-ray photoelectron spectroscopy (XPS) before and after deposition of Pt. From those analyses, we confirmed that strong metal support interaction (SMSI) between Pt and mesoporous metal oxides and significant changes of the electronic properties of Pt which could support the results of electrocatalytic activities.

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A Dual Amperometric/Potentiometric Microsensor for Simultaneous Measurements of Nitric Oxide and Calcium Ion

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Nitric oxide (NO) is known to be closely related to calcium ion (Ca^{2+}) in biological system. For instance, NO is continually produced by cNOS from blood vessels under normal condition. The activity of cNOS is dependent on calcium ion and calmodulin. Except for flow-dependent NO formation, there is basic pathway for the stimulation of cNOS, which involves release of calcium ions from subsarcolemmal storage sites. Endothelial receptors for a variety of ligands stimulate calcium ion release and generate subsequent NO production (receptor-stimulated NO formation).Due to this close linkage between NO and Ca^{2+}, it is of great interest to analyze NO and Ca^{2+} concurrently. In this presentation, we demonstrate the development of a dual microsensor for simultaneous measurements of NO and Ca^{2+} ion. A sensor possesses two microdisks: one disk is used for amperometric NO measurement and the other is used for potentiometric Ca^{2+} measurement. Sensor performances, such as sensitivity and selectivity, are characterized and the results show the possibility of the dual sensor for the biological applications. This research was supported by Basic Science Research Program through the National Research Foundation of Korea (NRF) funded by the Ministry of Education, Science and Technology (NRF-2011-0015619).

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Development of a needle-type dual electrochemical microsensor for real-time, simultaneous NO/CO measurements in dysfunctional rat brain

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Nitric oxide (NO) plays important role in regulating vasodilation in the brain. Carbon monoxide (CO) is also a physiologically important signaling molecule, which has analogous functions to NO. The exact functional relationship between NO and CO, however, has not been explained clearly yet, due to technical difficulties of measuring NO and CO simultaneously. To better understand the dynamic and close interactions of NO and CO, we fabricate an improved needle-type amperometric dual microsensor and optimize simultaneous monitoring of dynamic changes in NO and CO levels in vivo. The sensor consists of a planar working electrode possessing two Pt microdisks (diameter of each disk = 50, 76 μm) electrodeposited with second metals (Pt black, Au) and a Ag/AgCl reference electrode. Each disk surface of the working electrode is covered with gas permeable polymer membrane to obtain the selectivity to only NO or CO over common biological interfering species. The needle-shaped sensor allows to measure NO and CO underneath of the rat brain surface. The NO/CO dual sensor is applied to monitor dynamic changes of NO and CO levels in normal as well as dysfunctional rat brains. Our particular interest is to assess the effect of neuronal excitation in the interaction between NO and CO in acute seizure model. This research was supported by the National Research Foundation of Korea (NRF) grant funded by the Ministry of Education, Science and Technology (NRF-2011-0015619).

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Electrospun Titanium Oxide Nanofibers Decorated with RuO_2 Nanowires as a Highly Electrocatalytic Sensing Element

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Single crystalline ruthenium oxide nanowires were are successfully grown on electrospun titanium oxide nanofibers by simple thermal annealing (RuO_2 nanowires-TiO_2NFs). The morphology and structure of RuO_2 nanowires-TiO_2NFs were are characterized by field emission-scanning electron microscopy (FE-SEM). RuO_2 nanowires-TiO_2NFs are also characterized electrochemically. Compared to bare TiO_2NFs and $Ru(OH)_3$-TiO_2NFs electrode, The general electrochemical activity of RuO_2 nanowires-TiO_2NFs electrode represents faster electron transfer for the $[Fe(CN)_6]^{3-/4-}$ couple which are confirmed from the by cyclic voltammetry (CV) measurement and electrochemical impedance spectroscopy (EIS). Also, the amperometric response for the H_2O_2 oxidation and reduction is facilitated at the RuO_2 nanowires-TiO_2NFs electrode. This research was supported by the National Research Foundation of Korea (NRF) grant funded by the Ministry of Education, Science and Technology (NRF-2011-0015619).

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Synthesis and electrochemical characterization of ordered mesoporous cobalt stannides as anode for lithium-ion batteries

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Ordered mesoporous cobalt stannides (CoxSny) with various Co compositions are successfully synthesized through nano-replication technique as stable and high power anode materials for Li-ion battery. Especially, this is the first result for the synthesis of ordered mesoporous cobalt stannide through the direct template method. The electrochemical results show that meso-CoSn exhibits much better capacity than bulk CoSn. Reversible capacity, coulombic efficiency and cycle stability of mesoporous CoSn materials are dependent on their structure and composition. Especially, 30 atmic % Co contained ordered mesoporous cobalt stannide (refer to meso-CoSn-30) shows 83% capacity retention after 100 cycle, which means Co atoms effectively accommodate the volume strain associates with the lithiation?delithiation processes. Rate performance of 30 atmic % Co contained ordered mesoporous cobalt stannide are significantly improved, which was deeply related to the kinetic behaviors. Electrochemical impedance spectroscopy (EIS), galvanostatic intermittent titration technique (GITT) and ex-situ XRD (x-ray diffraction) experiments are carried out to gain the insight of the kinetic behaviors during the lithiation and delithiation processes. As a result, the low charge transfer resistance, large diffusion coefficient (small Warburg factor) and low internal resistance of meso-CoSn-30 moreover adequate amount of Co atoms contained to accommodate a volume fraction of Sn is the reason of cycle stability and superior rate capability.

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Effect of bilayered structure composed of TiO2 nanotubes and nanoparticles for dye-sensitized solar cells

강순형

전남대학교 화학교육과

Dye-sensitized solar cells (DSSCs) have been widely attracted due to low manufacturing cost, environmental friendliness, and high efficiency. However, there are still several drawbacks to attain the conversion efficiency above 15 % for the commercialization. In particular, in the photoanode comprised of TiO2 nanoparticles, the trap-limited diffusion process leads to the high charge recombination with a reduction of electron collection efficiency, even though it shows large surface area ensuring a high dye loading for light harvesting. One-dimensional TiO2 nanotube (TONT) by electrochemical two-step anodization in 0.25 wt% NH4F of ethylene glycol was suggested to overcome this problem. Herein, the overcoating of TiO2 nanoparticle was introduced to support the surface area because nanotubular structure has low surface area resulted from large inner diameter (approx. 100 nm) of nanotube. This bilayered TiO2 nanotube/nanoparticle film was characterized by XRD, FE-SEM, and J-V analysis.

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Inverse Opal SnO2 based sensitized solar cells

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전남대학교 화학교육과

Nowadays, the exploration of new photo electrode architectures to improve the light-harvesting and charge-collection properties of sensitized solar cells and related devices has been regarded as a challenging work. Here, we demonstrate the synthesis of the inverse opal SnO_2 film for sensitized solar cells by gravimetric sedimentation method, subsequently followed by the spin-coating or drop casting method. Using 430 nm poly styrene (PS) beads, we synthesized the SnO_2 inverse opal structure showing the photonic crystal effect. These results were confirmed using Field-emission scanning electron microscopy, X-ray diffraction and ultraviolet-visible spectrophotometer. Based on these results, SnO_2 inverse opal film was applied to sensitized solar cell to identify their unique properties and evaluated exploring the photocurrent-voltage measurement.

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Mussel-inspired functionalization of carbon nanotubes for synthesizing prussian blue-polydopamine-carbon nanotubes nanocomposites and its application for hydrogen peroxide sensing

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서울대학교 화학교육과

Mussel can attach itself to any kind of surface owing to its adhesive proteins which are similar to the functional groups of polydopamine (PDA). Inspired by mussel, a mild and environmentally friendly method was used to synthesize prussian blue(PB) on PDA coated carbon nanotubes. When dispersed in dopamine solution at room temperature, Multiwalled carbon nanotubes (MWNTs) were uniformly covered with PDA in consequence of the dopamine's one-step oxidative polymerization (PDA-MWNTs). PB-PDA-MWNTs nanocomposites could be synthesized by adding the PDA-MWNTs to an acidic solution of Fe^{3+}, $Fe(CN)_6]^{3-}$ and KCl in which PDA layer not only improved the dispersion of MWNTs in aqueous solution, but also was used as a platform for PB grafting. Combining MWNTs' excellent electronic properties and PB's high electrocatalytic activity toward H_2O_2 reduction, the MWNTs-PDA-PB modified glassy carbon electrode (MWNTs-PDA-PB/GCE) showed synergetic effect resulting in excellent ability as a hydrogen peroxide biosensor.

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Amperometric Biosensor Based on Covalently Immobilized Enzyme on Indium Tin Oxide (ITO) Glass Electrode

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연세대학교 화학과

Immobilization of enzymes on the electrode surface is a necessary and critical step in the design of biosensors. The covalent linkage of enzyme leads to high enzyme loading, increased stability and short response time of the enzyme electrode. An amperometric biosensor has been developed for the detection of phenols and glucose in aqueous solution. The enzyme, tyrosinase or glucose oxidase, was covalently immobilized on indium tin oxide (ITO) glass electrode using grafting method. The enzyme biosensor was prepared through reaction of enzyme with NHS-ester-grafted ITO glass, which was obtained by acid catalyzed reaction of NHS-ester-functionalized methallylsilane with ITO glass.In this study, the electrocatalytic responses of the enzyme modified biosensor for the detection of phenol and glucose were measured using both cyclic voltammetry and amperometry. Amperometric response was measured as a function of concentration of catechol and phenol, at applied potential of ?0.4 V versus Ag/AgCl in a phosphate buffer (pH 7.0). As a result, the present biosensor exhibited very fast response time of 1.3 s. In the glucose biosensor, electro-deposited platinum nanoparticles on electrode surface resulted in an efficient reduction of hydrogen peroxide, allowing the sensitive and selective quantitation of glucose by the direct reduction of enzymatically-liberated hydrogen peroxide at 0.4 V versus Ag/AgCl without a mediator.

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Fabrication of simple glucose biosensor with PtZn alloy electrode

김정현 **PIAOHUSHAN 손용근***

성균관대학교 화학과

Since 1990, the number of diabetic in Korea has maintained very high level. Moreover, the death rate of diabetic also evaluated as high in OECD nations. Therefore, it is important to test the level of glucose in the human blood. Various works for glucose sensors have been focusing on improving the sensitivity and selectivity. In this work, we fabricated PtZn alloy electrode for enhancing the surface area and choosing catalytic character to obtain simple glucose biosensor. We composed PtZn alloy by electrochemical deposition and disolution method and immobilized glucose oxidase on the surface by dropping method. After drying the glucose oxidase, nafion was coated on the surface for immobilization of glucose oxidase and exclusion of interference species like ascorbic acid and uric acid. As a result, we obtained a glucose biosensor with high sensitivity and selectivity. This work was supported by the Energy & Resource of the Korea Institute of Energy Technology Evaluation and Planning(KETEP) grant funded by the Korea government Ministry of Knowledge Economy(No. 2010501010002B)

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Improved electrochemical switching of ion transport

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성균관대학교 화학과

In our previous work, we controlled benzylamine(BA) transport through a conducting polymer modified membrane by applying various potentials. However, the transport rate was too low. Thus, we adopted a dual membrane system which can improve the transport rate and ion transport switching capability by applying electrical fields between two membranes. The membranes were prepared as following steps. First, gold was sputtered on the one side of the polycarbonate(PC) membrane and two membranes were overlapped PC side to PC side. Then, polypyrrole(PPy) was electrochemically deposited on the gold side of the two membranes, respectively. Finally, we controlled BA transport through this dual membrane system by applying potentials between two membranes and demonstrated the transport mechanism in detail. This work was supported by the Energy & Resource of the Korea Institute of Energy Technology Evaluation and Planning(KETEP) grant funded by the Korea government Ministry of Trade Industry and Energy(No. 2010501010002B)

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Non-enzymatic hydrogen peroxide sensor based on Polyaniline-MnO_2 nanocomposites modified electrode

이종혁 홍훈기*

서울대학교 화학교육과

Hydrogen peroxide is naturally produced by living organisms as a by-product of oxidative metabolism, therefore it is one of the most important analyte in various fields such as pharmaceutical, environmental and food analyses. There are many studies that determinate concentration of H_2O_2 based on enzyme using electrochemical methods. The enzyme-modified sensors has high selectivity and sensitivity. However, there are several disadvantages such as instability, high cost of enzyme, and temperature/pH-dependent operating condition. In this study, we synthesized polyaniline-MnO_2 nanocomposites by the simple mixing of aqueous dispersion of polyaniline(PANI) nanofibers and aqueous solution of $KMnO_4$. Subsequently, we fabricated PANI-MnO_2 nanocomposites modified electrodes by drop-casting method. It exhibited a good electrocatalytic effects in the reductions of H_2O_2. The non-enzymatic electrochemical sensors displayed high sensitivity, low detection limit and wide linear range.

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Layered graphene oxide/phosphorous nanocomposites for high capacity and cyclability anodes in lithium ion batteries

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Li ion battery(LIB)의 성능향상을 위한 많은 시도와 노력이 행해지고 있다. 본 연구에서는 큰 Li 저장용량을 갖는 것으로 알려진 phosphorus 와 graphene oxide(GO) nanocomposite 을 LIB 의 음극물질로 사용하여 높은 cyclability 를 보이는 고용량의 LIB 를 구현하고자 하였다. Phosphorus 는 제조 온도 및 압력에 따라 white phosphorus, black phosphorus, red phosphorus 3 가지 동소체로 나누어지며, 본 실험에서는 red phosphorus 를 선택하였다. 이는 white phosphorus 는 화학적으로 불안정하고, black 동소체는 열역학적으로 안정하나 합성하기 매우 어렵기 때문이다. Phosphorus 는 방전 시 3 V (vs. Li/Li^+)$3Li^+P?Li_3P$ 의 환원반응이 일어나며, 약 865mAh/g 의 이론용량을 가진다. 그러나 phosphorus 는 몇 cycle 지나지 않아 Li ion 의 intercalation/deintercalation 에 따른 부피변화로 인해 용량이 현저하게 감소되는 양상을 보이며, 이론용량과 큰 차이를 보인다. 본 연구에서 사용된 GO 는 phosphorous 에 의해 야기되는 stress 를 완충시키는 역할을 함으로서 음극의 안정성을 향상시킬 것으로 기대되었다. Nanocomposite 인 graphene oxide/phosphorus(GO/P)는 밀폐된 공간에서 phosphorus 를 400℃ 이상으로 가열함으로써 승화된 phosphorus 기체가 GO (또는 graphite oxide)와 균일한 혼합물을 형성하도록 하였다. 이후 X-ray diffraction(XRD)와 Raman spectrum 을 통하여 GO/P 가 합성되었음이 확인되었고, cell test 를 통하여 phosphorus 와 비교하여 합성된 GO/P 가 더 안정한 cyclability 와 용량 유지력을 갖는 것을 확인하였다.

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발표종류: 포스터, 발표일시: 수 16:00~19:00

Voltammetric detection of uric acid using immobilized uricase-Os complex on the SPCEs

조남현 김기훈[1] 우지현 최영봉 김혁한*

단국대학교 화학과 [1]단국대학교 나노바이오의과학과

Uric acid is purine derivatives, it is an organic compound consisting of carbon, oxygen, hydrogen, and nitrogen. Uric acid is derived from a purine located in the tissues most. Also, it increases the amount of urine excreted due to severe muscle movement or leukemia or burn. In addition, even at the onset of gout, the amount of uric acid in the blood and urine is increased. Electro-active complexes of osmium were prepared and then characterized using electrochemical techniques. Also, osmium complexs were prepared as a potential redox mediator in an bioelectrocatalytic system. The redox mediators presented here are described in shorthand as osmium complex which were immobilized with mixture onto the screen printed carbon electrodes (SPCEs). The electrical signals were measured by voltammetry techniques. Also, catalytical currents were amplified by uricase which is electrically mediated by new osmium redox complex, conversion the complex into an electrocatalysts for the electron reduction of oxidation of uric acid. The resulting catalytical currents were linearly related with the concentration of uric acid.

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발표종류: 포스터, 발표일시: 수 16:00~19:00

High sensitive electrochemical immunoassay for detecting hippuric acid using the new organic film that polymer-modified electrode which Ni^{2+} ion are attached

김남혁 이수정[1] 오인돈[1] 최영봉[1] 김혁한[1,*]

단국대학교 첨단과학대학 화학과 [1]단국대학교 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.For detecting HA, manufactured electrode immobilized Fe-HA complex on Ni^{2+} ion through the charge interaction.Hippuric acid (HA) has been detected competitively on the interaction of free HA and Fe-HA immobilized electrode to its antibody. The electrical signals proportional to the Fe-HA was monitored by cyclic voltammetry (CV) and differential pulse voltammetry (DPV). The surface morphology of the immobilized Ni/Fe-HA on the carbon electrode was examined by scanning electron microscopy (SEM) and X-ray Photoelectron Spectroscopy (XPS). The proposed electrochemical immunoassay method can be extended to various applications for detecting a wide range of different small antigens in the health care area.

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Electrochromic properties of flexible porous Lithium doped Nickel oxide films by simple wet-coating method

정영희* 김영일[1]

(주)마프로 기술연구소 [1]부경대학교 화학과

Nickel oxide is well known inorganic electrochromic material. The size, morphology and electrochromic performance of NiO films are affected by precursor, temperature and concentration. In this study, NiO and lithium doped NiO particles were synthesized by chemical precipitation with various precursor and heat treatment at 400℃ for 3h. Flexible NiO and Lithium doped NiO(Li-NiO) films on ITO/PEN substrate were prepared by wet coating method using an alcoholic solution that have a porous structure. Li-NiO films showed improved coloration efficiency compared to the undoped NiO films. Complimental electrochromic device was assembled by combination of the Li-NiO and WO3 electrodes with a gel electrolyte. Li-NiO/gel electrolyte/WO3 device showed the electrochromic color change between transparent and greenish brown. The response time for bleaching and coloring was found to be 4.4s and 18s respectively.

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

Observation of potential controlled current responses in single Pt nanoparticle collisions on Ni ultramicroelectrode

정아람

건국대학교 화학과

Collisions of several kinds of metal or metal oxide single nanoparticles (NPs) with a less catalytic electrode surface have been observed through amplification of the current by electrocatalysis. Two general types of current response, a current staircase or a current blip (or spike) are seen with particle collisions. The different current responses are depended on the NP collision and electrocatalytic reaction mechanism. The current staircase is due to the electrocatalytic current increase whenever the collided NPs are sticked on the electrode. On the other hands, the reason of current blip is believed as the NP attachment and following deactivation process. We observed the current response of single NP collision is controllable from staircase to blip by changing the deactivation process. We investigated the relationship between current response and the deactivation process using a system consist of platinum (Pt) NP collision and the nickel ultramicroelectrode(UME). The current response of Pt NP observed as staircase on the 0 V (vs. Ag/AgCl) applied nickel UME and as blip on the 0.12 V (vs. Ag/AgCl) applied nickel UME.

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발표종류: 포스터, 발표일시: 수 16:00~19:00

Ion Conduction in Cucuirbituril-based Organic Porous Materials

박준혁 김기문* 윤민영[1]

포항공과대학교 화학과 [1]가천대학교 글로벌캠퍼스 화학과

Developing highly efficient devices for energy storage and conversion such as fuel cell and lithium ion battery is necessary. As ion conducting materials determine not only operation condition, but also efficiency of such devices, development of a new ion conducting material is crucial to make better energy converting devices. Hydrogen fuel cell requires development of proton conducting materials with high proton conductivity, whereas leak free lithium conducting solid materials are required in LIB for safety issue. Herein, we report a new organic molecular porous solid, porous cucuirbit[6]uril (CB[6]), and its remarkable ion conducting properties. The porous CB[6] has a honey-comb-like structure with 1D cylindrical channels (channel size: 7.5 ?). The channels were filled with water and acid molecules, forming a hydrogen bonded network. Interestingly, single crystal conductivity measurement revealed highly anisotropic proton conductivity of the porous CB[6] (????||/ ????⊥ ~8600) and showed high proton conductivity of 1.3?10-3 S?cm-1. For better understanding the anisotropic proton conduction behaviors, motion of protons in the channels of the porous CB[6] was studied using solid state 2H-NMR spectroscopy. The NMR study suggested that an anisotropic proton motion is dominant at low temperature (

Ion Conduction in Cucuirbituril-based Organic Porous Materials

박준혁[1,2] 서경원[1] 윤민영[1,2] 김기문[1,2,3*]

IBS 복잡계 자기조립 연구단,[1] 포항공과대학교 화학과,[2] 첨단재료과학부[3]

Developing highly efficient devices for energy storage and conversion such as fuel cell and lithium ion battery is necessary. As ion conducting materials determine not only operation condition, but also efficiency of such devices, development of a new ion conducting material is crucial to make better energy converting devices. Hydrogen fuel cell requires development of proton conducting materials with high proton conductivity, whereas leak free lithium conducting solid materials are required in LIB for safety issue. Herein, we report a new organic molecular porous solid, porous cucuirbit[6]uril (CB[6]), and its remarkable ion conducting properties. The porous CB[6] has a honey-comb-like structure with 1D cylindrical channels (channel size: 7.5 Å). The channels were filled with water and acid molecules, forming a hydrogen bonded network. Interestingly, single crystal conductivity measurement revealed highly anisotropic proton conductivity of the porous CB[6] ($\sigma_{\parallel}/\sigma_{\perp}$ ~8600) and showed high proton conductivity of $1.3 \cdot 10^{-3}$ $S \cdot cm^{-1}$. For better understanding the anisotropic proton conduction behaviors, motion of protons in the channels of the porous CB[6] was studied using solid state ^{2}H-NMR spectroscopy. The NMR study suggested that an anisotropic proton motion is dominant at low temperature (<373 K). In addition, it can be extended to lithium ion conductor for an application in LIBs. We used the channels of guest-free porous CB[6] as a conduction pathway of lithium ions. This lithium doped porous organic materials showed low activation energy (0.32 - 0.4 eV) and 10^{-5} $S \cdot cm^{-1}$ of lithium ion conductivity.

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Synthesis of Ru-on-Pd Nanochain Networks and Their Application as Electrocatalysts for Oxygen Reduction Reaction

정인택 심준호*

대구대학교 화학·응용화학과

This presentation reports the facile synthesis and characterization of carbon-supported Ru layer-coated Pd nanochain networks (Ru-on-PdNN/C). A series of Ru-on-PdNN/C with various Ru/Pd weight percentage ratios were prepared by the spontaneous deposition of a Ru cluster on a Pd nanochain networks core using different Ru precursor concentrations. The compositional/structural features were characterized by scanning electron microscopy (SEM) equipped with an energy dispersive X-ray spectroscopy (EDS), high-resolution transmission electron microscopy (HRTEM), X-ray diffraction (XRD), and X-ray photoelectron spectroscopy (XPS). The electrocatalytic activity of the Ru-on-PdNN/C for oxygen reduction reaction (ORR) in alkaline media was measured by RDE polarization experiments. Indeed, the prepared Pd based nanocatalysts, especially the Ru-on-PdNNs decorated with a very low amount of Ru, exhibited significant electrocatalytic activity toward the ORR. This activity is critically dependent upon the Ru coverage on a Pd core surface. This research was supported by a grant of the Korea Sanhak Foundation (2013).

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Tailoring Au-core Pd-shell Nanoparticles Supported on Reduced Graphene Oxide for Enhanced Electrocatalytic Activity

노성민 심준호*

대구대학교 화학·응용화학과

In this work, we have demonstrated the synthesis and characterization of non-platinum bimetallic AuPd nanoparticles supported on reduced graphene oxide (AuPd/RGO). AuPd/RGO catalysts are prepared by a simple synthetic method of RGO-supported Pd-coated Au nanoparticles via a spontaneous reduction of Pd(II) to Pd(0) on a Au nanoparticle surface without a treatment with any additional reducing agent. The compositional/structural features are characterized by scanning electron microscopy (SEM) equipped with an energy dispersive X-ray spectroscopy (EDS), high-resolution transmission electron microscopy (HRTEM), X-ray diffraction (XRD), and X-ray photoelectron spectroscopy (XPS). The electrocatalytic activity of the AuPd/RGO for oxygen reduction reaction (ORR) in alkaline media was measured by RDE polarization experiments. The catalytic activity of AuPd/RGO is comparable to the commercial Pd-20/C and Pt-20/C catalysts. This activity is critically dependent upon the Pd-shell coverage and thickness on a Au core surface. This research was supported by a grant of the Korea Sanhak Foundation (2013).

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발표종류: 포스터, 발표일시: 수 16:00~19:00

Electrocatalytic Activity of Nanoporous RuPd Nanoparticles in Oxygen Reduction

조승기 심준호*

대구대학교 화학·응용화학과

We have rationally synthesized and optimized catalytic nanoparticles consisting of a Pd core, partially covered by a Ru shell. The amount of Ru used is extremely small, yet they show unusually high activity for electroreduction of oxygen. The optimized structure has only ultra-low content of Ru (<0.1 mM of RuCl3) but a further increase in the loading of Ru will actually reduce catalytic activity, inferring that a synergistic effect exists between the two different metal nanostructure components. A combined electrochemical and spectroscopic study of oxygen reduction reaction (ORR) reveals that Pd-core Ru-shell-cluster nanostructure has some unique electronic and morphological properties. The structures and electrocatalytic activities of the nanoporous RuPd catalysts are characterized by scanning electron microscopy (SEM) equipped with an energy dispersive X-ray spectroscopy (EDS), transmission electron microscopy (TEM), X-ray diffraction (XRD), X-ray photoelectron spectroscopy (XPS), cyclic voltammetry (CV), and rotating disk electrode (RDE) voltammetry. This research was supported by a grant of the Korea Sanhak Foundation (2013).

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발표종류: 포스터, 발표일시: 수 16:00~19:00

Alloy Pt-Co electrocatalyst supported on thiolated graphene oxide for oxygen reduction reaction

윤미라 전승원*

전남대학교 화학과

Alloy PtCo nanoparticles electrocatalyst-supported thiolated graphene oxide (tGO) was synthesized (PtCo/tGO) in an easy and fast way for an efficient oxygen reduction reaction (ORR). After electrochemical reduction of PtCo/tGO (ER/PtCo/tGO), ER/PtCo/tGO was characterized by scanning electron microscope (SEM), transmission electron microscope (TEM), X-ray photoelectron spectroscope (XPS), energy dispersive spectroscope (EDS) and electrochemical impedance spectroscope (EIS). Electrocatalytic activities were verified by cyclic voltammetry (CV), rotating ring disk electrode (RRDE) in 0.1 mol L-1 KOH aqueous solution, which is also used to assess the catalyst's kinetic parameters. The ER/PtCo/tGO catalyst shows exceptionally high catalytic performance, with its electrocatalysis of O2 reduction reaction via four-electron transfer reduction to H2O.

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Different length linkages of carbon-supported silver nanoparticles for oxygen reduction reaction in alkaline media

이경미 전승원*

전남대학교 화학과

Different length linkages of carbon-supported silver composites were prepared by a two step synthesis method. To investigate the relationship between the linker length and the catalytic activities of the metal decorated GO catalysts, three sample were prepared with three different linker molecules, HS(CH2)2SH, HS(CH2)3SH and HS(CH2)4SH (denoted as GO-l-NPs) and silver nanoparticles. This sample were tested in oxygen reduction reaction (ORR) using electrochemical techniques such as cyclic voltametry (CV) and rotating ring disk electrode (RRDE) hydrodynamic voltametry to quantitatively obtain the ORR kinetic constants and the reaction mechanisms on a glassy carbon electrode (GCE) in 0.1M NaOH solution. All GO-l-Ag/GCE electrodes showed significantly improved ORR activity mechanisms. GO-l-Ags were characterized by X-ray photoelectron spectroscopy (XPS), transmission electron microscopy (TEM) and scanning electron microscope (SEM). The results showed that silver were successfully attached onto the GO surface. A more positive potential catalytic ORR was observed in the modified GO-l-Ags with shorter chain linker lengths.

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Pd nanoparticles supported on PEDOT functionalized graphene oxide for oxygen reduction reaction

최주은 전승원*

전남대학교 화학과

Pd nanoparticles supported on PEDOT functionalized graphene oxide [Pd/PEDOT/rGO] was prepared using chemical method. Pd/PEDOT/rGO was characterized via field emission scanning electron microscopy (FE-SEM), X-ray photoelectron spectroscopy (XPS), energy dispersive X-ray spectroscopy (EDS) and electrochemical impedance spectroscopy (EIS). The electrochemical properties and electrocatalytic O2 reduction of Pd/PEDOT/rGO are evaluated via cyclic voltammetry (CV) and rotating ring disk electrode (RRDE) in 0.1 M KOH aqueous solutions. The results show that Pd/PEDOT/rGO demonstrates excellent catalytic activity for oxygen reduction.

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A biosensor using a biomimic membrane comprising Cytochorme C

이민영 김동민 심윤보*

부산대학교 화학과

A biosensor based on Cytochrome C (Cyt C) comprised biomimic membrane has been study to detect superoxide radical(O_2 ??) and peroxynitrite(ONOO?). The membrane was constructed using Cyt C/Fe_2O_3 /lipid on a conducting polymer layer poly(2,2’:5’,2”-terthiophene-3’-p-benzoic acid (poly-TTBA)) formed on the Au nanoparticles, deposited-screen printed electrode. The characteristics of the biomimetic layers were investigated by cyclic voltammetry, linear sweep voltammetry, SEM and XPS analyses. Cyt C with lipids (Phosphatidic acid (PA),and Cardiolipine (CL)) and Fe_2O_3 were involved in electron transfer sequence in the sensor probe. The redox peak potentials of the Cyt C/ Fe_2O_3 modified electrode were observed at 0.11V(Epc)/0.66V(Epa) (vs. Ag/AgCl) in a 0.01M PBS (pH 7.4). In the case of the Cyt C/ Fe_2O_3 /lipids (PA or CL), a pair of redox peak ere appeared at 0.14V(Epc)/0.75V(Epa) with PA, whereas Epc/Epa are 0.16V/ 0.67V at CL. The electron transfer rate constants for biomimic membrane were determined to be 0.686 s?^{1} .

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니오븀계 음극 활물질의 전자상태 해석 및 전기화학적 특성 평가

유찬서 김양수* 황선호[1]

한국기초과학지원연구원 순천센터 [1](주)유림산업 기술연구소

고용량·고안정성 전극으로서의 가능성을 지닌 재료로 Nb 계 산화물이 있으며, 기존의 탄소재료를 능가 할 수 있는 특성을 가지고 있는 것이 확인되었다. 당 연구팀은 $Li_{1.1}Nb_{0.9}O_{2-y}$ 을 리튬 이차 전지의 음극용 신규 활물질로 제안하였다. 본 물질은 제 1 원리계산을 통해 선택하였고, 고상법으로 합성에 성공하였다. 제 1 원리 계산 결과 $Li_{1.1}Nb_{0.9}O_{2-y}$ 재료에서 일어나는 리튬 이온의 산화환원 반응은 낮은 전위에서 일어날 것으로 예측 했으며, 전기화학적 측정에 의해 실험적으로 확인되었다. 하지만 $Li_{1.1}Nb_{0.9}O_{2-y}$ 의 용량은 기대치보다 작아 이 원인을 찾기위하여 결정구조를 달리하는 $Li_{1.1}V_{0.9}O_{2-y}$(R-3M)과 $Li_{1.1}Nb_{0.9}O_{2-y}$(P63/mmc)를 가지고 전자상태계산을 수행하였다. 전자상태 계산은 $(Li_{13}Nb_{12}O_{62})^{73-}$와 $(Li_{17}Nb_{20}O_{48})^{14-}$ 클러스터 모델을 사용하여 DV-X_{α} 법을 이용하여 화학결합을 가지고 검토하였다. Mulliken 해석으로 $Li_{1.1}V_{0.9}O_{2-y}$(R-3M)과 $Li_{1.1}Nb_{0.9}O_{2-y}$(P63/mmc)의 Li 전하와 Li-O 와 V-O 에 대한 공유결합성을 검토하였다.

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Graphene/conducting polymer gel based hybrid material for oxygen reduction

AZADUDAYPRATAP 심윤보*

부산대학교 화학과

Graphene and 1,8-diamininaphthalene based graphene-conducting polymer gel material was prepared. The prepared materials was characterized by Raman spectroscopy, transmission electron microscopy (TEM), scanning electron microscopy (SEM), cyclic voltammetry, powder X-ray diffraction (XRD) and X-ray photoelectron spectroscopy (XPS). Further the electrochemical properties of the prepared material were explored for oxygen reduction reaction (ORR) using cyclic voltammetry, electrochemical impedance spectroscopy (EIS) and hydrodynamic voltammetry at optimized experimental condition. Chronoamperometry and chronocoulometry was also performed for the estimation of kinetic parameters for ORR.

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An Electrochemically Prepared poly (diaminonapthalene/Graphene) material as metal free catalyst for oxygen reduction reaction

MALENAHALLIHALAPPANAVEEN 심윤보*

부산대학교 화학과

Introducing nitrogen functionalities containing conducting polymer with carbon materials can be a powerful path to find an alternative catalyst for oxygen reduction reaction (ORR) which can replace the expensive Platinum (Pt) catalyst. Here we report a simple electrochemical method to approach ORR with a metal free electrocatalyst, prepared by uniform incorporation of diaminonaphthalene monomer with graphene oxide through electropolymerization process. The resulting material was characterized by X-ray photon spectroscopy (XPS) and morphological studies has done by using FE-SEM, and TEM images. Electrochemical measurements were carried out to measure the ORR activity by cyclic voltammetry in alkaline solution. For further insight into electron transfer parameters of poly (diaminonapthalene/Graphene), the RDE experiments were performed at different rotation speeds. These results indicate an acceptable increased current density with mainly a 4 electron transfer process, long term stability, and superior methanol tolerance, as compare to the of commercially available Pt/C catalyst.

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Transmission Electron Microscope Analysis of Recovering Lithium from Bittern by Electrochemistry Process

최윤주 유찬서 김양수*

한국기초과학지원연구원 순천센터

The lithium is used in very wide field, but the whole amount of lithium resources from the land is limited and on this point it will be very important and urgent of all the nations to have a security of the lithium supply as a energy source for the future. So in this context the research is going on for the stable supply of the lithium from the bittern. Generally, the lithium manganese oxide showed a topotactic extraction of Li^+ in the aqueous phase largely through an ion-exchange mechanism, and the Li^+ extracted samples indicated a high selectivity and a large capacity for Li^+. In the process of extraction reaction, we applied to collected Li_2O, not the existing Li_2CO_3. In this study, we experimented a microstructure observation in all-solid-state battery with Li_2O composite positive electrode during charge-discharge process.This idea has been supported by measurements of the general method using neutron diffraction of Li_2O by T.W.D Farley et al,. This indicates that the existence of a disordered fast-ion phase within Li_2O suggested by measurements of the self-diffusion coefficients of Li_2O. Consequently, Our group showed good results for lattice planes, fringe distances compared by T.W.D Farley et al,.

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FeF_3/activated carbon foam (ACF) nanocomposites with enhanced electrochemical performance as a cathode material for lithium-ion batteries

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Lithium-ion batteries (LIBs) have high operating voltage, high energy density, low self-discharge ratio, and long cycle lifetime. However, further researches to develop LIBs with enhanced reversible lithium-storage capacities are still necessary for their widespread applications in electric vehicles and energy storage systems. The specific capacities of LIBs are mainly limited by their electrode materials, especially the cathode side. Therefore, development of cathode materials with a higher theoretical capacity is needed. FeF_3 is one of the promising cathode materials because of its low cost, safety, and environmental friendliness compared to commercialized $LiCoO_2$. In addition, FeF_3 has a theoretical capacity of about 237 and 712 $mAhg^{-1}$ at 2.0-4.5 and 1.5-4.5 V, respectively. These capacities are higher than that of $LiCoO_2$ (a reversible capacity of 140 $mAhg^{-1}$). However, FeF_3 has drawbacks of poor electrical conductivity and sluggish lithium-ion diffusion, which lead to its inferior cycle retention and rate capability. In this study, FeF3 nanoparticles were impregnated into the mesopores of activated carbon foam (ACF) and crystallized inside the pores through the calcination under argon where ACF was utilized as both a template and a conductive agent. The synthesized FeF3/ACF nanocomposites were thoroughly characterized by BET, XRD, SEM, and TEM. The nanocomposites exhibited the improved electrochemical performances. For example, they delivered high discharge capacities of about 195 and 468 $mAhg^{-1}$ at 0.1 C in the voltage ranges of 2.0-4.5 V and 1.5-4.5 V, respectively. Their capacity fading rate was observed to be about 0.4 %/cycle at 2.0-4.5 V, which is superior to that of bare FeF_3. All the cell tests were conducted at room temperature.

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Facile Synthesis and Electrochemical Performance of Carbon-Coated V_2O_5 Nanoparticles Using Organic Acid as a Carbon Source for Li-Ion batteries

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Vanadium pentoxide (V_2O_5) with a layered structure has been considered as a promising cathode material for Li-ion batteries (LIBs) because of its low cost, abundance, and relatively high theoretical capacity (about 294 $mAhg^{-1}$ at 2.1-4.0V), compared with more commonly used cathode materials such as $LiCoO_2$ (140 $mAhg^{-1}$) and $LiFePO_4$ (170 $mAhg^{-1}$). However, V_2O_5 has disadvantages of its poor structural stability, low electrical conductivity, and sluggish diffusion of Li ion, resulting in poor cycling stability and rate performance. In this work, V_2O_5 nanoparticles coated by carbon layer with a thickness of approximately 3-6 nm are synthesized via a facile thermal-decomposition of vanadium precursor ($(NH_4)(VO)C_6H_5O_7$) where citric acid ($C_6H_8O_7$) is used as both a carbon source and a chelating/reducing agent. Furthermore, the synthesized carbon-coated V_2O_5 nanoparticles have a loosely porous microstructure which originates from the interspaces between the aggregated particles. This V_2O_5 sample exhibits a high initial discharge capacity of about 293 $mAhg^{-1}$ between 2.1-4.0 V at 0.1 C rate and capacity retention of about 90 % after 30 cycles. At high current densities in the range of 0.1-5.0 C, the excellent rate capability and cycling stability are also achieved. The effects of citric acid on the electrochemical performance of V_2O_5 are thoroughly compared by using oxalic acid ($C_2H_2O_4$) and tartaric acid ($C_4H_6O_6$) in the place of citric acid.

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Observation of signal change in single Ag nanoparticle collisions on Au ultramicroelectrode by oxidation of Ag nanoparticle

이상민

건국대학교 화학과

Collisions of silver nanoparticles (Ag NPs) with a more?electrocatalytic gold (Au) electrode surface have been observed. In contrast with previous observations of single NP collision, less electrocatalytic material is employed as a NP and more electrocatalytic material is employed as an electrode. The Au ultramicroelectrode(UME)?shows better electrocatalytic activity than the Ag for the hydrazine oxidation reaction. Therefore, when the Ag NP collides on to the Au UME, the electrocatalytic current of hydrazine oxidation by the Au UME are hindered by collided Ag NP. The catalytic current decrease was observed as staircase response as like as previous single NP collision experiments. In addition, when the higher potential which is above the Ag oxidation potential was applied to the Au electrode, collision signal was changed?from staircase to blip response. It may be due to the Ag?NPs?on the electrode are?oxidized and recovered the electrode?surface.?We investigated the current response of single Ag NP collision on the Au UME with various applied potential using electrochemical methods.

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Size dependent separation of gold nanoparticles using an electrochemical micro?uidic channel

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The size separation of gold nanoparticles (AuNPs) from mixed samples has been studied based on an electrochemical potential modulated microfluidic channel (EPMM). The separated sizes of AuNPs (dia. 5, 25, 50, and 75 nm) were substantiated by UV-visible spectroscopy, cyclic voltammetry (CV), and transmission electron microscopy (TEM). The experimental parameters that affected the EPMM based separation and detection of AuNPs was studied in terms of AC amplitude, AC frequency, ?ow rate, concentration (mg/ml), sample volume (μl) and detection potential. The separated particles were collected individually at the end of the micro channel and the separation efficiency was evaluated with the retention time and peak area.

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Effects of graphene oxidation in SnO2 graphene composite anode materials for Li-ion batteries

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다양한 종류의 Li ion battery anode 물질이 graphene 과 전이금속 산화물의 결합을 통해서 연구되어 지고 있다.하지만 현재 그래핀의 산화정도가 이 물질에 주는 영향에 대한 연구는 미비한 상황이다.이에 그래핀을 산화시키는 정도를 차이를 주고, SnCl4 5H2O 를 결합시켜서 그래핀과 SnO2 물질이 결합된 형태의 anode 물질을 합성하였다.이를 구조적, 전기화학적으로 연구하여 그 특성 차이를 연구하였다.결과적으로 그래핀의 산화정도에 따라서 SnO2 graphene anode 물질의 용량과 용량 감소 차이가 생겼으며, 이 차이를 연구하였고, 이러한 차이가 나오는 원인에 대해서 결과를 도출해 내었다

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Synthesis of various metal oxides functionalized by conductive materials for high performance pseudocapacitor

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We introduce a facile method to synthesize metal oxides such as NiO, CuO, and MnO2 with hierarchical structure, and to improve the pseudocapacitor properties of metal oxides by simply depositing conductive materials. Supercapacitors could be categorized in two types; electric double layer capacitor (EDLC) and pseudocapacitor depending on charge absorption mechanism to the active material surface. Pseudocapacitors, which utilize metal oxides as active materials, store the charges by physical adsorption and chemical redox reactions, resulting in high capacitance values than EDLC. However, they suffer from several problems such as poor stability and low conductivity. In this study, we improve the capacitance properties via synthesizing hierarchical 3D structure and physical doping of conductive materials.

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Ascorbic Acid Detection with Hollow Gold/Ruthenium Nanoshells by Amperometry

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Hollow gold/ruthenium (hAu-Ru) nanoshells were prepared by the hybridization of Ru on hollow gold (hAu) nanoshells synthesized from Co nanoparticle templates. The hAu-Ru nanoshells represented catalytic effect on ascorbic acid (AA) oxidation without any interference from glucose, acetamidophenol, uric acid and dopamine at the proper potential which was determined by analyzing linear sweep voltammograms. The structure and spectroscopic properties were identified by FE-SEM, HR-TEM, XRD, XPS and Raman spectroscopy. Amperometric current responses showed selective and stable current response toward AA oxidation on hAu-Ru modified electrode without aid of enzyme. Moreover, the practicability of this sensor was verified with recovery test of AA in real samples (urine and vitamin C tablets). The hAu-Ru modified electrode showed sensitivity of 426 μA $mM^{-1}cm^{-2}$ for the linear dynamic range of zero to 2 mM AA with the response time of 1.6 s and detection limit of 2.2 μM.

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Electrocatalytic Properties of Hollow AuPd Nanoshells

이다은 조아라 이영미* 이종목*

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We synthesized the hollow AuPd nanoshells (hAuPd) via a two-step galvanic replacement reaction (GRR) using the Co nanoparticles (Co NP) as a template. The hollow Au nanoshells (hAu) were prepared via GRR between Co NP and Au precursor. Again, hAu was galvanic exchanged with various concentrations of Pd precursor (x, y, and z mM) to obtain hAuPdx, hAuPdy and hAuPdz, respectively. The structure and morphology of hAuPds were characterized by scanning electron microscopy (SEM), transmission electron microscopy (TEM), X-ray diffraction pattern (XRD), X-ray photoelectron spectroscopy (XPS) and UV-vis spectroscopy. The rotating disk electrode (RDE) experiments at hAuPdy modified on glassy carbon electrodes in alkaline media showed enhanced performance of oxygen reduction reaction (ORR) compared to commercial Pt. The amperometric H_2O_2 reduction was conducted at physiological pH (7.40) and showed that the activity increased as the content of Pd increased. Furthermore, the interference of other species (i. e. glucose, ascorbic acid, acetamidophenol, uric acid and dopamine) in physiological condition was completely blocked. Cyclic voltammetry (CV) was also performed for the ethanol oxidation in alkaline media to confirm a possibility of application to direct alcohol fuel cell (DAFC).

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Electrochemical characterization of ALP-pNPP reaction on multilayered gold nanoparticle electrodes

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경북대학교 화학과

본 포스터에서는 탄소 칩 기반의 전극에 layer by layer(LbL) 공법을 이용하여 금 나노입자와 alkaline phosphatase(ALP)를 정전기적으로 고정하고 이들 효소의 생활성도를 기질인 para-nitrophenylphosphate(pNPP)와 반응시켜 전기화학 신호를 측정한 결과를 발표하고자 한다. 특히 공유결합을 통해 고정한 ALP 효소 전극과 LbL 공정법에 의해 제작된 전극에서의 ALP 효소반응의 특성, 효율성 및 재현성을 비교분석한 전기화학적 분석 데이터를 나타냈다.

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Sodium and calcium ion selective sensors using micro-liquid/gel interfaces

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본 포스터는 서로 섞이지 않는 두 전해질 (수용성 액체/유기성 젤) 계면에서 소듐 이온과 칼슘 이온의 보조 전이 이동 반응에 따라 전류값의 변화에 기초를 둔 센서의 개발에 관한 결과를 나타냈다. 소듐 및 칼슘 이온과 각 각 선택적으로 착물을 잘 형성하는 이온운반체인 dibenzo-18-crown-6 와 ETH 129 를 유기성 젤에 도포하여 이들 리간드에 도움을 받아 각 이온이 물층에서 유기층으로 이동할 때 이동한 이온의 양에 따라 전류값이 비례하여 변화하는 것에 기반을 둔 센서로 계면 한 개당 두 개의 이온운반체를 칵테일로 사용할 경우 두 이온을 동시에 검출할 수 있음을 확인하였다. 순환전압전류법(Cyclic voltammetry)과 시차펄스 벗김 전위법(Differential pulse stripping voltammetry)을 사용하여 얻은 정량적인 전기화학적 데이터를 보여주고자 한다.

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F- anion selective sensors with micro-liquid/gel interfaces

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본 포스터 발표에서는 플로라이드 이온선택성 리간드를 이용해 플로라이드 음이온을 전기화학적 방법으로 검출하고자 하였다. 물과 1,6-dichlorohexane/polyvinylchloride 를 이용해 만든 액체-유기성 계면에서 플로라이드 이온의 이동 반응을 전기화학적으로 조사하고 이에 따른 전류값 변화를 측정함으로써 F- 음이온을 정량 분석하고자 하였다. 먼저 액체-젤 계면에서의 플로라이드 음이온의 직접적인 이동 반응을 순환 전압전류법으로 측정한 결과 리간드가 없는 액체-젤 계면에서 플로라이드 이온의 이동 반응은 관찰되지 않았다. 플로라이드 이온선택성 리간드가 있는 젤 층에 도포되어 형성한 액체-젤 계면에서는 플로라이드 음이온이 물 층에서 유기 층으로 그리고 유기 층에서 물 층으로의 이동함에 따라 전류값이 변화함을 관찰하였다. 플로라이드 음이온의 농도 변화에 따라 전류값이 증가함을 측정한 예비 데이터를 통해 플로라이드 선택적 센서의 제작이 가능함을 보여주고자 한다.

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Single Piece All-Solid-Contact Lead(II)-Selective Electrode Based on copoly(Aniline-Aminoquinoline) Particles with Intrinsic Conductivity

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Novel concept of a single-piece all-solid-state ion selective electrode (SPE) is introduced. A processable conducting polmer (CP) is dissolved in a cocktail containing the components used for a ion selective membrane. The cocktail solution, containing the CP, is cast directly on a solid substrate (Platinum), resulting in a SPE. The role of the CP is to mediate the charge transfer between the substrate and the membrane. A new ion selective membrane electrode was facilely prepared by using aminoquinoline copolymer micropatricles with an intrinsically electrical conductivity as a lead (II) ionophore. It found that the electrode performance will significantly be improved by changing the aniline and amioquinoline ratio. The aniline and aminoquinoline (80:20) copolymer are found to optimal electrode for lead (II) ion. The optimal electrode has an excellent selectivity of lead (II) ion over alkali, alkaline earth and other transition metal ions.

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Scale-up flow type microbial fuel cells for waste water treatment and energy generation

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Two large volume microbial fuel cells (MFC) with different structural designs have been constructed and tested in both batch and continuous flow modes to compare waste treatment ability and energy generation efficiency. A tubular-type cell with volume of 393 mL comprised a rolled carbon cloth anode (20 cm x 40 cm) and a stainless steel mesh-based air cathode (18 cm L x 5 cm diameter) loaded with 0.3 mgcm-2 Pt/C catalyst. A rectangular shape MFC with 2 L volume (30 cm L x 10 cm W x 6 cm H) was constructed by placing three reticulated vitreous carbon (RVC) anodes (9.5 cm x 5.5 cm x 0.5 cm each) equally distanced from each other, and eight stainless steel mesh based-cathodes (6 cm x 5 cm each) with 0.3 mgcm-2 Pt/C catalyst that were diagonally placed with respect to the anode. The maximum power density of the cylinder-type cell was 7.9 W/m3 at 24 hydraulic retention time with current density of 17.2 Am-3 at maximum power density. A rectangular cell produced maximum power density of 3.5 Wm-3 at 2 mLmin-1 flow rate with current density of 10 Am-3 at the maximum power point. The power density dropped to 2.2 Wm-3 at current density of 7.5 Am-3 after shifting to the batch mode operation.

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Structural and Electrochemical Characterization of Proton Irradiated Graphene Oxide

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동국대학교 화학과

Studies on improvement of the characteristic properties of graphene oxide through investigation on chemical and electrochemical modification using proton beam. Assesment of the physical properties such as thermal conductivity, withstanding voltage, thermal stability via the modification and control of mophological and electrochemcal propropeties of graphene oxide irradiated by proton beam. Studes on interfacial nature, diffusion and charge transfer kinectics of graphene oxides irradiated by proton beam using impedance spectroscopy and cylic voltammetry in various electrolytes. Strucutral and Physical analysis of graphen oxide irradiated by proto beam using XRD, SEM, TEM, IR, elementaly analysis, and thermogravimetry.

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Visible Light Energy Harvesting via Light Trapping Effect of Three-layered Hybrid TiO_2 Structure for Photoelectrochemical Water Splitting

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Energy harvesting via visible light which occupies almost half of whole sun light is very important issue for many applications where sun light is utilized. We made a very efficient three-layered structure to trap the light in the TiO_2 (titanium dioxide) nanostructures. It contains a square patterned P25 layer, a thick P25 layer and a mesoporous TiO_2 inverse opal layer which serves as antireflection layer, a light absorption layer and a reflecting layer, respectively. CdSe quantum dots which have small band gap energy were attached on the surface of the nanostructure to excite electrons via photon trapping. This structure can be broadly used for efficient energy materials with photonic properties.

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Nanographene-decorated avidin layer on electrode surfaces as an electrochemical sensing platform

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Avidin was modified on indium tin oxide (ITO) electrode surfaces through charge interaction. Then graphene oxide (GO) sheets were deposited on the avidin-modified ITO surfaces, which was followed by an electrochemical reduction of GO for preparing electrochemically reduced graphene oxide (ERGO)-modified ITO surfaces. After an immobilization of biotinylated probe biomolecules on the avidin binding sites, the resulting surfaces were employed as sensing platforms for electrochemical detection of target molecules. For enhancing the performance of the sensor, an electrocatalytic activity of ERGO toward redox active molecules such as benzoquinone was employed in electrochemical measurements. In this contribution, we present an optimization procedure of the sensor platform for the sensitive detection, and demonstrate a high efficiency of the platform.

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전해질과 이온 개념에 대한 중학생의 개념생태 특징

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이 연구는 중등학생들이 전해질과 이온 개념 형성에 어려움을 겪고 있는 이유를, 학습자의 인지적 측면뿐만 아니라 정의적, 심리적 측면에서 살펴보고자 개념 생태적 접근을 통하여 개념생태 요소를 조사한 것이다. 중학교 3 학년 남학생 1 개 반과 여학생 1 개 반을 연구 대상으로 사전과 사후의 개념 검사, 과학태도 검사, 교사와 학생 심층 면담, 수업관찰, 노트, 교사의 학생 프로파일 등을 통하여 연구 자료를 수집하였다. 연구 결과는, 첫째, 학생들은 중학교 2 학년 과정에서 이미 학습한 원자, 원소, 이온의 개념이 형성되지 않고 있었으며 이것은 이온의 이동이나 전해질에 대한 개념을 학습하는데 제한점으로 작용하고 있었다. 둘째, 중학생들의 교실 수업 문화는 수동적인 것으로 나타났으며 수업 참여도는 남학생 반과 여학생 반에서 매우 다른 수업 분위기를 형성하고 있었다. 셋째, 교사의 일방적인 전달식 수업은 빠른 시간 안에 많은 양의 내용을 제공하고, 이것은 학습자들이 스스로 학습에 대한 어려움 또는 학습능력 부족으로 인식하게 하였다. 넷째, 중학생들의 전해질과 이온 개념을 구성하는 개념생태 요소는 인식론적 확신 근거, 정의적 영역, 비유, 과거 경험 등으로 나타났다. 중학생들의 전해질과 이온에 대한 개념생태 연구의 결과는 중학생 수준에 있어서의 전해질과 이온 단원에 대한 보다 실질적인 교수전략을 모색하는데 시사점을 제공할 수 있을 것이다.

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창의성 유형별 PBL에서 나타나는 창의적 문제해결 과정

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본 연구는 문제중심학습(PBL)에서 창의성 유형에 따라 창의적 문제해결 과정에서 나타나는 차이점을 비교하였다. P 고등학교의 과학영재학급 학생을 대상으로 TTCT 도형검사를 사용하여 적응적 창의성 유형과 혁신적 창의성 유형으로 분류하였다. 3 가지 PBL 문제를 개발하여 문제중심학습 모형을 사용한 9 차시 수업을 투입하여 창의성 유형별로 문제해결 과정에서 보이는 특징을 살펴보았다. 수업장면의 녹화 및 녹음, 성찰일기 작성, 인터넷 카페의 댓글 활동 관찰을 통해 자료를 수집하였다. 연구 결과, 문제중심학습의 단계마다 창의성 유형별로 창의적 문제해결 과정에서 서로 다른 양상을 나타내는 것을 살펴볼 수 있었다. 문제 알아가기 단계에서는 적응적 창의성 유형의 학생들은 경청하는 자세를 보였고, 혁신적 창의성 유형의 학생들은 산만한 태도를 보였다. 문제 재정립하기 단계에서는 적응적 창의성 유형의 학생들은 정교성과 제목의 추상성을 사용하여 현재의 패러다임을 유지하기 위해 노력하며 문제에 접근하였고, 혁신적 창의성 유형의 학생들은 독창성과 유창성을 발휘하여 문제가 지닌 가정에 의문을 품었다. 정보 찾아보기 단계에서는 적응적 창의성 유형의 학생들은 정교성과 제목의 추상성을 이용하여 효율적이며 조직적인 과정을 통해 문제해결에 필요한 정보를 수집하였고, 혁신적 창의적 유형의 학생들은 독창성과 유창성을 발휘하여 새롭고 다양한 시각에서 정보에 접근하였다. 문제 해결하기 단계에서는 적응적 창의성 유형의 학생들은 제목의 추상성과 정교성을 바탕으로 신중한 태도로 효율적이고 조직적 방법으로 문제를 해결해나갔고, 혁신적 창의성 유형의 학생들은 독창성과 유창성을 이용하여 비효율적이거나 독창적인 방법으로 문제를 해결하였다. 마지막 공유와 평가하기 단계에서는 적응적 창의성 유형의 학생들은 문제해결의 내용에 초점을 두었고, 혁신적 창의성 유형의 학생들은 학습지의 형식에 관심을 갖고 장난으로 행동하는 경우도 있었다.

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교과교실 활용 원리를 적용한 과학과 교과교실제 수업의 효과

홍미영

한국교육과정평가원 교수학습개발본부

본 연구에서는 선행 연구(홍미영, 송현정, 김천홍,2011)에서 제시한 교과교실 수업 원리 4C(Creativity, Critical thinking,Communication, Cooperation)를 바탕으로 수업안을 개발하여 실험적으로 10 주 동안 적용해 봄으로써 교과교실 운영상의 효과와 적용상의 제한점을 탐색하였다. 교과교실 원리 활용 수업의 효과는 수업안 적용 전후의 학생들의 교실 학습환경 인식과 정기고사 성적 변화로 알아보았다. 연구 결과, 수업 처치에 따른 가시적인 학생들의 학습환경 인식 변화는 나타나지 않았다. 실험 적용 전후에 각각 실시한 중간고사와 기말고사 성적에 대하여 통제 집단과 실험 집단 간 독립평균차이검정을 실시한 결과 두 집단 간에 통계적으로 유의미한 차이는 없었다. 이 결과는 수업 진도의 압력에도 불구하고 교사 수준 교육과정 재구성을 통해 비판적 사고력, 창의성, 협동성 등을 구현하는 활동 중심의 과학 수업의 가능성을 시사한다는 점에서 긍정적이라고 볼 수 있다.

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다문화탈북 가정 학생의 과학 학업성취도 특성 및 화학 문항 분석

김현경

한국교육과정평가원 교육평가본부

본 연구에서는 전수로 시행된 국가수준 학업성취도 평가의 중학생 과학 성취도를 다문화탈북 집단별 성취특성, 문항별 집단별 정답률 및 변별도, 내용영역별, 정답률 차이가 큰 문항유형별 특성을 계량적, 질적 방법으로 분석하였다. 연구 결과, 다문화탈북 가정 학생의 과학과 학업성취도는 일반 학생에 비해 매우 낮았으며, 기초학력과 기초미달 학생의 비율이 매우 높았다. 또한 다문화탈북 가정 학생의 하위집단별로 과학과 학업성취도가 다르게 나타났으며, 특히 중도입국 학생과 탈북 가정 학생의 학업성취도가 가장 낮았다. 일반 학생과의 정답률 차이가 큰 문항을 분석한 결과, 중도입국 학생과 탈북 가정 학생의 경우는 전 영역에서 고루게 취약한 반면, 외국인 가정 학생의 경우는 특정 영역에서 취약함을 보였다. 이로부터 다문화탈북 가정 학생을 위한 교수학습 및 교육 지원이 각각 집단의 상황을 고려하여 적합한 방식으로 이루어지도록 교육적 함의를 도출하였다.

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2009 개정 교육과정에 따른 국가수준 학업성취도 평가를 위한 화학 성취기준 및 세부성취기준 개선

김현경

한국교육과정평가원 교육평가본부

이 연구는 학업성취도 평가의 성공적인 시행을 위하여 2009 개정 교육과정을 반영하여 중학교 과학의 학업성취도 평가를 위한 성취기준과 세부성취기준을 개선하였다. 이를 위해 2007 개정 교육과정과 2009 개정 교육과정을 분석하고, 2009 개정 교육과정에 따른 중학교 핵심 성취기준을 분석하고, 국가수준 학업성취도 평가의 기존 성취기준을 분석하였다. 이를 토대로 2009 개정 교육과정에 따른 국가수준 학업성취도 평가를 위한 성취기준과 세부성취기준을 개선하고 이에 따른 예시 문항을 개발하였다. 이 연구는 궁극적으로 국가수준 학업성취도 평가 시행을 위한 토대를 마련할 뿐만 아니라 체계적이고 타당한 학업성취도 평가 체제를 구축함으로써 국가 수준의 성취수준 및 추이 결과 산출, 보고 등의 신뢰성 제고와 학교교육 성과를 진단하여 추후 교육과정 개발에 필요한 정보를 제공하는데 시사점을 얻을 수 있다.

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암실 속 과학 활동에 대한 과학교육자, 특수교사, 장애학생의 반응

김학범 박승재[1] 차정호*

대구대학교 과학교육학부 [1]대구대학교 사범대학 물리교육과

이 연구에서는 암실 환경에서 진행된 과학체험 활동에 대한 과학교육자, 특수교사, 그리고 장애학생의 반응을 비교하였다. 세 집단을 대상으로 진행된 체험 활동에서 설문지와 면담을 통해 자료를 수집하였다. 체험 전 과학에 대한 인식과 장애 관련 체험 경험등에 대한 사전 질문을 한 뒤, '물의 구조' 및 '눈의 구조와 기능'과 관련된 모형을 암실 환경에서 스스로 체험하도록 하였다. 체험하는 동안 생각하는 것을 질문함으로써 학습 진행 과정을 점검하였고, 활동이 끝난 뒤 느낀 점을 물었다. 인터뷰 내용을 전사하여 세 집단간 특징을 추출하고, 이를 비교하였다. 세 집단(과학교육자, 특수교사, 장애학생)간의 특징 비교를 통하여 시각장애 학생의 과학교육에 대한 시사점을 도출할 것이다.

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STEAM형 마인드맵을 적용한 중학교 2학년 학생들의 창의적 사고력 신장

유현정 강순희*

이화여자대학교 과학교육과

이 연구에서는 STEAM 형 마인드맵을 활용한 창의적 문제해결력 지향 교수 전략을 개발하고 한 학기 동안 중학교 2 학년 학생들에게 적용하여 창의적 사고력 신장 측면에서 그 효과를 검증하고자 하였다. STEAM 형 마인드맵이란 하나의 과학 주제와 관련된 아이디어들을 과학측면(S), 기술측면(T), 공학측면(E), 예술측면(A), 수학측면(M)으로 생각해보고 펼쳐보는 발산적 활동이다. 다양한 측면(S, T, E, A, M)으로 생각을 확장하도록 의도적으로 유도하면서 창의적인 사고를 지향하는 점이 기존의 마인드맵과의 두드러진 차이라고 할 수 있다. 이 연구에서는 창의적 사고력을 발산적 사고로 협의적으로 정의하였고 그 하위 범주로 유창성, 융통성, 독창성의 신장을 보았다. 또한 학업성취도 수준, 인지 수준, 학습 스타일에 따라 창의적 사고력의 신장을 알아보았다. 그 결과 창의적 사고력에서 유의미한 신장이 나타났으며 하위 범주 중에는 유창성, 독창성에서 통계적으로 유의미한 신장을 나타내었다(p

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과학 글쓰기를 통한 중학교 3학년 학생들의 전해질에 대한 이해 분석

이규희 홍훈기*

서울대학교 화학교육과

이 연구에서는 설명하여 글쓰기와 상상하여 글쓰기로 구성된 과학 글쓰기 과제를 이용하여 '전해질과 이온' 단원의 이해도 및 과학 글쓰기에 나타나는 특성을 분석하였다. 또한, 선택형, 서술형 문항으로 구성된 혼합형 과제와 과학 글쓰기에서 나타난 결과를 비교해 보았으며, 과학 글쓰기에 대한 학생들의 인식을 조사 하였다.과학 글쓰기 과제 및 혼합형 과제는 중학교 3 학년 '전해질과 이온' 단원을 목표 단원으로 하였다. 혼합형 과제는 선행연구(이순희, 2002) 및 한재영 등(2006)이 개발한 자료에서 관련 있는 문항만을 추출하여 변형 없이 사용하였으며, 이와 같은 내용으로 과학 글쓰기 과제를 개발하였다. 개발된 과제는 예비 연구 및 현직 교사와 과학 교육 전공자와의 세미나를 통해 수정, 보완 하여 최종 연구에 사용 하였다.서울시에 소재한 중학교 3 학년 학생 12 명을 대상으로 하였다. 이들은 모두 관련 단원을 학습한 상태였다. 과학 글쓰기 활동 후, 혼합형 과제를 제시하고 완성하게 하였다. 활동에 참여한 전체 학생들을 대상으로 개인면담을 실시하였다. 면담의 공통질문은 과학 글쓰기 활동 후 학생들의 인식을 묻는 문항들로서, 선행연구(구슬기, 2010)에 사용된 면담 질문들 중 연구의 목적에 맞는 것만을 추출하여 사용하였으며, 과학 글쓰기와 선택형 문항에서 서로 다른 결과를 보인 학생들에게는 추가 질문을 포함하여 면담을 시행하였다.연구 결과, 과학 글쓰기에서는 과학적 개념을 가진 것으로 조사된 학생이 선택형 문항에서는 오답을 선택하거나, 과학 글쓰기에서 정확한 과학적 개념을 가지지 않은 것으로 조사된 학생이 선택형 문항에서 정답을 선택하기도 하였다. 또한, 학생들은 서술형 문항에서보다 과학 글쓰기에서 평균적으로 더 많은 과학 용어를 이용하는 것으로 나타났다. 면담에서, 대부분의 학생들은 과학 글쓰기가 과학 학습에 도움을 주며, 흥미 있는

과정이라고 응답하였으며, 꾸준히 학습 하고자 하는 의향을 보였다. 그러나 실제 수업 시간에서 활용 시, 수업 진행이 어려울 것 같다는 응답을 한 학생도 있었다.

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중, 고등학교 과학 실험실 환경 및 과학 교사들의 안전 교육에 관한 인식조사

김현영* 이재환 류재정[1]

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3 차 교육과정 이후 탐구활동을 중요시 하는 것이 과학교육의 중요한 목표로 자리 잡고 있다. 탐구활동에서 많은 비중을 차지하는 실험활동은 여러가자 안전사고를 수반하고 이를 예방하기 위한 많은 노력을 기울이나 사고의 비율은 해마다 증가하고 있다. 사고원인의 대부분은 학생 부주의가 많았다. 그러므로 안전교육을 실시하는 교사들의 안전의식을 고취시키는 것은 중요하다. 그래서 본 연구에서는 현재 중, 고등학교 화학 실험을 하는 교사들의 안전 의식 실태와 실험실 환경을 알아보고자 일선 학교 현장의 40 여명 과학 교사들에게 설문조사를 실시하였다. 선행 연구 조사를 바탕으로 만들어진 설문조사는 실험실의 일반적인 환경 및 사고에 대비한 준비, 안전한 실험을 위한 개인보호 장비, 폐기물 처리 방법 및 지식, 약품에 관한 지식과 취급 능력, 사전 실험 실태, 사고에 대비한 응급처치 능력, 안전교육 실태 및 필요성과 효과를 조사항목으로 설정하였다. 설문조사 결과 실험실 환경은 교사들의 기대에 미치지 못하는 수준이었고, 화재및 안전사고가 방생했을때 대비할 수 있는 환경 역시 제대로 갖추어져 있지 않았다. 실험실 안전을 위한 학생들의 교육 및 교사들의 교육 또한 부족하고 교육을 위한 자료 역시 부족하였다. 본연구를 통해서 교사들의 실험실 안전의식을 고취시키기 위해서 다양한 자료와 프로그램의 개발과 실험실 안전에 실질적인 도움을 줄수 있는 연수이 필요성을 언급하고, 교육 현장에 체계적이고 효율적인 실험실 안전교육의 근간을 마련하기 위한 토대를 제공하고자 한다.

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발표종류: 포스터, 발표일시: 수 16:00~19:00

중학교 2학년을 대상으로 한 과학 교과서 내 탐구활동 App. 개발 및 적용

이창윤 홍훈기[*]

서울대학교 화학교육과

이 연구에서는 스마트기기를 활용한 탐구활동의 효과를 학업성취도, 과학적 태도, 과학에 대한 흥미 측면에서 알아보았다. 연구 대상은 중학교 2 학년 학생 70 명이었으며, 실험반 35 명과 통제반 35 명이 연구에 참여하였다. 목표 단원은 2009 개정 중학교 2 학년 과학 교과서의 '물질의 구성' 단원으로 하였다. 연구에 사용된 탐구활동 App.은 연구자가 Action Script 3.0 을 통해 직접 개발하였고, 과학 교육 전문가, 현직 교사, 과학교육 전공자와의 세미나를 통해 수정, 보완하여 최종 연구에 사용하였다. 실험반 학생들은 스마트기기를 활용한 탐구활동 수업에 참여했으며, 통제반 학생들은 App.의 구성 내용을 탐구활동지로 받고 수업에 참여했다.

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별도 교육 방식이 아닌 정규 과학 수업에서의 중학교 1학년 학생들의 논리 사고력 신장

홍혜인 강순희*

이화여자대학교 과학교육과

본 연구에서는 비례, 보존, 변인 통제, 확률, 상관, 조합 논리 활동을 강화한 교수 전략을 경험한 학생들이 그러한 교수 전략을 경험하지 못한 학생들에 비해 논리적 사고력이 향상될 것이라고 설정하였다. 학생의 인지 발달을 가속시키기 위한 프로그램인 CASE 프로그램을 적용한 기존 연구들을 살펴보면 구체적 조작 후기 단계와 형식적 조작 초기 단계 즉 주로 초등 학생들에게서 인지 가속 효과가 특히 크게 나타난 것으로 보고되고 있다. 따라서 본 연구에서는 별도의 교육 프로그램이 아닌 정규 과학 수업에서의 논리 활동 강화 수업 전략을 개발하였으며 개발한 수업 전략의 효과를 알아보기 위하여 초등 4, 5, 6 학년과 비슷한 인지 수준 분포를 보이는 서울 소재 중학교의 1 학년 학생 총 110 명을 대상으로 60 차시 동안(1 학기 중간고사 이후부터 2 학기 기말고사 전까지) 수업을 진행하였다. 57 명의 실험 집단의 학생들에게는 교과서 중심의 비례, 보존, 변인 통제, 확률, 상관, 조합 논리 활동을 강화한 논리 사고력 수업을 진행하였으며 53 명의 통제 집단의 학생들에게는 교과서 중심의 일반적인 탐구 수업을 실시하였다. 그 결과 논리 사고력에서 실험 집단과 통제 집단에서 통계적으로 유의미한 차이가 있었으며 특히 구체적 조작기와 과도기 학생에게 유의미한 신장이 나타났다. 6 개의 하위 논리 유형 형성에 대한 분석 결과 비례 논리, 확률 논리, 상관 논리를 제외한 보존 논리와 변인통제 논리, 조합 논리, 전체 합계에서 그 차이가 통계적으로 유의미하였다.

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초·중등학생의과학캠프를 통해 본 나노화학에 관한 인식 연구

추교찬 고원배[1,*]

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2009 개정 교육과정에 맞추어 개편된 과학 교과서에서 나노화학에 대한 초중등학생의 인식을 조사했다. 수업을 효과적으로 진행하기 위해 필요한 기초자료를 자체 제작하여 학생들에게 제시했다. 서울시 노원구청 주관과 삼육대학교 나노무기화학연구실 주최로 노원구 거주 초·중등학생 92 명을 대상으로 실험진행에 대한 설문조사를 실시하였다. 그 결과는 다음과 같다. 첫째, 학생들의 나노화학에 대한 관심도는 긍정적이었고, 나노화학에 대한 개념의 내용과 실험은 신비하고, 재미있다고 대답하였다. 초등학교 저학년 학생 일수록 여러가지 나노화학 실험중 나노 섬유실험에 높은 관심을 보였고 , 나노과학분야의 물질개발에서 새로운 나노입자 합성에도 관심을 많이 가졌다. 둘째, 학생들의 나노지식에 대한 인지도와 나노과학 관련 지식에 대한 이해도는 실제 높은편은 아니었다. 학생과 교사 모두 다양한 경로를 통하여 나노화학에 대해 접했던 것으로 조사되었다. 셋째, 초·중등학생은 대부분 대학과 연계 수업을 매우 선호했고, 많은 기대를 하고있었다. 나노수업이 필요하다는 점에 대해서는 공감하고 있었다. 초중학생들이 체험교재를 통해 실험한 결과 특히 풀러렌을 직접 만들고 연꽃잎 효과와 나노섬유, 산환 환원반응에 대한 체험학습을 선호했다.

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물질의 상태변화에 대한 중학생의 성취수준별 문제 해결 능력

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우리나라는 2008 년부터 국가수준 학업성취도 평가를 이용하여 교육과정 수준에서 학생들의 교육 목표 도달 정도를 확인해오고 있다(김동영 외, 2012). 국가수준 학업성취도 평가의 연구보고를 통해 우리나라 학생의 평균적인 능력을 이해할 수 있으며, 성취 수준별로 문항별 학생의 정답률과 오답의 빈도 등의 정보를 알 수 있다. 그러나 성취도 평가 결과는 학생들이 왜 정답을 찾지 못하는가에 대한 정보를 제공하지는 못하고 있다. 교과교실제와 수준별 이동 수업의 요구가 점차 확대되고 있는 현 교육 상황에서 성취수준별 학생들에 대한 미시적인 정보를 도출하여 학교 현장에 제공할 필요가 있다. 본 연구는 상태변화에 대한 중학교 1 학년 학생들의 성취수준별 문제해결능력의 차이를 알아보는 데 목적이 있다. 이를 위해 이미 국가수준 학업성취도 평가에서 타당도와 신뢰도가 검증된 문항을 활용하여 설문과 면담을 실시하였다. 상태변화의 용어, 상태변화 시 입자모형에 대한 성취도 문항을 이용하여 성취수준에 따라 정답률과 오답률을 분석하고, 그들의 반응에 대한 이유를 분석하였다. 상태변화의 용어와 관련된 문항에서는 우수학력의 경우 문제해결에 어려움이 없었으나, 기초학력이나 보통 학력의 경우 응결상황에서의 상태변화에 대하여 인식에 어려움을 가지고 있었다. 이들은 김을 기체라고 인식하여 기화라고 응답하는 비율이 높았으며, 이는 응결 상황 자체가 아니라 제시된 맥락에 초점을 맞추어 인식하기 때문으로 보였다. 한편 기초미달의 경우, 상태변화에 대한 용어를 정확히 모르고, 잘못된 사례를 암기하고 있어 문제해결에 어려움이 있었다. 액체 아세톤의 기화와 관련된 상태변화 문항의 해결에 있어서는 우수학력이나 보통학력은 입자적 관점으로 문제해결이 잘 되었으나, 기초학력이나 기초 미달 학생의 경우, 상태변화 시 분자 수가 증가하여 부피가 증가하는 것이라는 인식을 드러냈다. 이들은 입자는 작아지면서 수가 증가한다고 생각하여, 액체 입자와 기체 입자를 다른 것으로 인식하고 있었다. 또한 아세톤의 기화를 확산으로

설명하는 경우가 있었다. 상태 변화에 대한 학생들의 문제해결 방식은 성취수준에 따라 고유한 특성을 가지고 있었다. 이는 성취수준별 학생의 교수학습에 있어 시사점을 제공할 수 있을 것이다.

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온도에 따른 기체의 부피변화에 대한 중학생의 성취수준별 이해 분석

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우리나라는 2008 년부터 국가수준 학업성취도 평가를 이용하여 교육과정 수준에서 학생들의 교육 목표 도달 정도를 확인해오고 있다(김동영 외, 2012). 국가수준 학업성취도 평가의 연구보고를 통해 우리나라 학생의 평균적인 능력을 이해할 수 있으며, 성취 수준별로 문항별 학생의 정답률과 오답의 빈도 등의 정보를 알 수 있다. 그러나 성취도 평가 결과는 학생들이 왜 정답을 찾지 못하는가에 대한 정보를 제공하지는 못하고 있다. 교과교실제와 수준별 이동 수업의 요구가 점차 확대되고 있는 현 교육 상황에서 성취수준별 학생들에 대한 미시적인 정보를 도출하여 학교 현장에 제공할 필요가 있다. 본 연구는 온도에 따른 기체의 부피변화에 대한 중학교 1 학년 학생들의 성취수준별 문제해결능력의 차이를 알아보는 데 목적이 있다. 이를 위해 이미 국가수준 학업성취도 평가에서 타당도와 신뢰도가 검증된 문항을 활용하여 설문과 면담을 실시하였다. 성취수준에 따라 정답률과 오답률을 분석하고, 그들의 반응에 대한 이유를 분석하였다. 뜨거운 물에서 찌그러진 농구공이 팽팽해지는 현상에 대하여 대부분의 학생들의 분자운동이 활발해지기 때문이라는 정답의 선택률은 매우 높았으나, 이유에 대한 서술을 분석한 결과 다양한 학생들의 응답유형이 파악되었다. 우수학력의 경우, 온도가 높아져서 분자운동이 활발해지고, 분자의 농구공에 면에 충돌 수가 증가하여 압력이 증가하여 부피가 증가하였다는 논리적인 순서로 설명한 빈도가 많았다. 그러나 성취 수준이 낮을수록 온도가 높아 분자운동이 활발해지고, 부피가 증가하였다는 식의 더욱 단순한 설명이 많아졌다. 일부는 부피가 늘어나서 분자운동이 활발해졌다고 진술하여 논리의 순서가 제대로 되지 않은 경우도 있었다. 한편, 기초학력과 기초미달 학력의 경우, 분자크기의 증가와 분자 수의 증가로 인해 활발해져

부피가 늘어났다고 인식하는 경우도 있었다. 온도에 따른 기체의 부피 변화에 대한 학생들의 이해 양상은 성취수준에 따라 고유한 특성을 가지고 있었다. 이는 성취수준별 학생의 교수학습에 있어 시사점을 제공할 수 있을 것이다.

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2007 개정 교육 과정 중학교 과학3 교과서 '전해질과 이온' 단원 내용의 인지 요구도 수준 분석

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본 연구는 2007 개정 교육 과정에 의한 중학교 과학 3 교과서 '전해질과 이온' 단원의 내용에 대한 인지 요구도 수준을 분석하고 중학교 3 학년 학생들의 인지 수준을 조사하였다. 이를 통해 교과서의 내용이 학생들의 인지 수준에 맞게 서술되었는지 알아보고 학생들이 어려워하는 개념을 파악하고 효율적인 학습을 위한 교과 내용 재구성에 도움을 주고자 하였다. 교과서의 인지 요구도 수준 분석은 CSMS 프로그램에 의해 개발된 CAT 분류틀을 사용하였으며 '전해질과 이온' 단원의 내용을 4 개의 주요 개념(전해질과 비전해질, 이온화, 화학 반응식, 앙금 생성 반응)으로 분류하고 개념 별로 「탐구 활동」과 「본문 내용」으로 나누어 실시하였다. 인지 수준은 중 3 학생 151 명을 대상으로 GALT 축소본을 사용하여 조사하였다. 연구 결과를 요약하면 다음과 같다. 첫째, '전해질과 이온' 단원의 전해질과 비전해질의 「탐구 활동」은 전해질과 비전해질을 단순히 분류하므로 대부분의 교과서에서 최상위 인지 요구 수준이 후기 구체적 조작기(2B)이다. 교과서 C 는 이온의 개념을 포함하여 최상위 인지 요구 수준이 초기 형식적 조작기(3A)이다. 「본문 내용」은 전해질을 구분하고 STS 로 설명한 교과서 B, E, F, I 의 경우 초기 형식적 조작기(3A)가 최상위 인지 요구 수준이며, 전해질을 단순히 분류한 교과서 A, C, D, G, H 는 후기 구체적 조작기(2B)가 최상위 인지 요구 수준이다. 둘째, 이온화의 「탐구 활동」과 「본문 내용」은 이온의 개념과 모형에 대한 이해가 필요하므로 대부분의 교과서에서 최상위 인지 요구 수준이 초기 형식적 조작기(3A)이다. 교과서 D, E 의 「탐구 활동」은 실험 설계의 내용을 포함하여 최상위 인지 요구 수준이 후기 형식적 조작기(3B)이다. 셋째, 화학 반응식의 「탐구 활동」과 「본문 내용」은 이온화 과정을 화학 반응식으로 나타내어 모든 교과서에서 최상위 인지 요구

수준이 초기 형식적 조작기(3A)이다. 넷째, 앙금 생성 반응의 「탐구 활동」과 「본문 내용」은 앙금 생성 과정을 모형과 화학 반응식으로 나타내어 6 종의 교과서에서 최상위 인지 요구 수준이 초기 형식적 조작기(3A)이다. 교과서 B, E, I 의 「탐구 활동」은 실험 설계의 내용을 포함하고, 교과서 E, I 의 「본문 내용」은 조합 논리를 사용하여 최상위 인지 요구 수준이 후기 형식적 조작기(3B)이다. 다섯째, ‘전해질과 이온’ 단원의 「탐구 활동」과 「본문 내용」의 인지 요구 수준을 비교해보면 전해질과 비전해질에서는 「탐구 활동」이 더 낮은 인지 수준을 요구하는 교과서가 많으며 나머지 주요 개념은 비슷하다.

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중학교 과학3 '물질의 특성' 단원의 내용 인지 요구도 수준 분석

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본 연구의 목적은 학생들의 인지 발달 수준과 교과 내용의 인지 요구도 수준이 불일치할 때, 효율적인 학습이 어렵다는 피아제의 이론을 근거로 하여 2007 개정 과학과 교육 과정의 중학교 3 학년 ‘물질의 특성’ 단원의 내용 인지 요구도 수준과 국내의 중학교 3 학년 학생들의 인지 수준을 비교·분석해 보고자 함이다. 본 연구의 분석 결과를 요약하면 다음과 같다. 첫째, 피아제의 발달 단계에 따르면 중학교 3 학년 학생들은 형식적 조작기에 도달했어야 한다. 그러나 GALT 축소본을 사용한 연구를 문헌 조사한 결과, 모집단 별로 차이가 있지만 최소 27.4%에서 최대 44%의 학생만이 형식적 조작기에 도달하였다. 둘째, 주요 개념 별로 영국의 CSMS Project Team 의 CAT 분류틀을 사용하여 본래 개념과 교과서의 내용 인지 요구도 수준을 분석한 결과는 다음과 같다. ‘크기 성질 및 세기 성질’은 후기 구체적 조작(2B) 수준의 개념이다. 다음으로 ‘밀도’ 개념은 초기 형식적 조작(3A) 수준이나 교과서에서는 본문 내용은 최고 수준으로 초기 형식적 조작(3A) 수준, 탐구 활동은 후기 형식적 조작(3B) 수준을 요구한다. ‘끓는점과 어는점 및 녹는점’은 초기 형식적 조작(3A) 수준인 개념이다. ‘용해도’는 초기 형식적 조작(3A) 수준인 개념이지만 교과서에서 본문 내용은 최고 수준으로 초기 형식적 조작(3A) 수준, 탐구 활동은 후기 형식적 조작(3B) 수준을 요구하였다. 마지막으로 ‘혼합물의 분리’는 초기 형식적 조작(3A) 수준인 개념이고 교과서에서도 대체로 동일한 수준을 요구하였다. 위와 같은 결과를 종합하여 얻은 결론은 다음과 같다. 중학교 3 학년의 ‘물질의 특성’ 단원은 대체로 초기 형식적 조작(3A) 수준으로 서술되었고, 이는 대체로 교과서의 서술 방식의 차이보다는 개념 자체의 특수성이 원인이 된 인지 수준이다. 일부 중학교 3 학년 학생들은 형식적 조작기에 미치지 못해 이를 이해하기 어려울 수 있다. 그러나 교과서를 쉽게 서술하기 보다는 이들의 인지 수준을 높이는 데에 노력을 기울여야 하며, 학습자의 인지 수준과 교과 내용의 인지 수준이 반드시

일치해야만 학습이 일어나는 것은 아니므로 이해에 어려움을 겪는 학생들의 경우 효과적인 교수-학습 모형이나 비유, 다양한 실례 등을 활용하면 도움이 될 것이다.

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열과 우리 생활 그리고 분자 운동과 상태 변화의 평가 문항 인지 요구도 수준 분석 - 2009 개정 과학①

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본 연구는 2009 년 개정 과학과 교육 과정의 과학① 교과서에서 화학 관련 영역인 ‘분자 운동과 상태 변화’ 와 내용상 연계되어 있는 ‘열과 우리 생활’ 단원을 선정하여 해당 교육 과정 9 종의 교과서를 본문 문항과 마무리 문항으로 나누어 Lawson 의 평가 문항이 요구하는 인지 수준 분류틀로 인지 요구도 수준을 판정해 보았다. 본 연구 결과를 요약하면 다음과 같다. 첫째, 9 종 교과서의 ‘열과 우리 생활’ 단원 마무리 문항에서 가장 많은 비율의 ‘가설-연역적 인지 수준(HD; Hypothetical-Deductive)’을 요구하는 교과서는 I(78.6%)로 9 종 교과서의 평균(56.1%)보다 훨씬 높았으며, 가장 적은 교과서는 F(36.3%)로 I 교과서와 큰 차이를 나타냈다. ‘분자 운동과 상태 변화’ 단원 마무리 문항 역시 ‘가설-연역적 인지 수준(HD)’의 비율이 가장 높은 교과서는 H(77.8%)이며, 가장 적은 교과서는 A(36.4%)이다. Lawson 의 SRT 검사를 통한 중학교 1 학년 학생들의 인지 수준이 ‘경험-귀납적’ 55.6%, ‘과도기’ 37.2%, ‘가설-연역적’ 7.3%로 가설-연역적 인지 수준이 가장 적게 나타났던 것을 감안한다면, H 와 I 교과서는 평가 문항이 학생들의 인지 수준과 매우 큰 차이를 보인다. 둘째, 해당 교육 과정의 9 종 교과서에서 전체 평가 문항 수가 적게는 46 개(H 교과서), 많게는 107 개(A 교과서)로 매우 다양하게 나타나며 본문 문항의 평균 문항수가 마무리 문항보다 많은 것으로 나타났다. 셋째, ‘열과 우리 생활’과 ‘분자 운동과 상태 변화’ 단원의 본문 문항과 마무리 문항의 인지 요구도 수준을 11 개의 하위 요소로 분석해 본 결과 ‘열과 우리 생활’ 단원의 평가 문항 중 ‘특정 사실의 기억(R; only the Recall of specific facts)’, ‘경험-귀납적 인지 수준(EI; Empirical-Inductive thinking pattern)’의 하위요소인 ‘EI4’와, ‘가설-연역적 인지 수준(HD; Hypothetical-Deductive)’의 하위 요소인 ‘HD1’, ‘HD3’ 수준은 모든 9 종의

교과서에서 나타나고 있으며, 가장 높은 비율을 차지하고 있는 하위수준은 'HD1' 과 'EI4' 이다. 넷째, 2009 개정 과학과 교육 과정에서는 창의적 문제 해결력을 강조하고 있으나, 2007 개정 교육 과정에 해당하는 중학교 2 학년의 '열에너지' 단원과 교과서들을 비교해 봤을 때 '열과 우리 생활' 단원에서는 오히려 '특정 사실의 기억(R)'을 요구하는 평균 문항 비율이 17.1%에서 29.8%로 높아지고, '가설-연역적 인지 수준(HD)'을 요구하는 평균 문항 비율은 51.4%에서 36.4%로 크게 줄어든 것으로 나타났다.

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과학과(화학영역) 교육과정 개정에 따른 교과서 삽화의 변화 및 학습효과에 미치는 영향 분석

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과학과(화학영역) 교육과정 개정에 따른 교과서 삽화의 변화를 조사하였다. 과학과(화학영역)에 포함된 삽화의 종류, 소재 및 역할을 비교·분석하였으며, 삽화 역할의 유형을 세분화하였다. 삽화의 종류는 사진, 그림, 도해, 만화, 도표 및 기타로, 삽화의 소재는 과학적 상황, 자연적 상황 및 생활적 상황으로, 삽화의 역할은 동기유발, 실험안내, 자료제공, 실험결과 제시 및 기타로 분류하였다. 중, 고등학교 학생들을 대상으로 삽화에 대한 인식 및 학습효과에 미치는 영향을 조사하고, 분석하여 효과적인 삽화활용을 위한 자료로 제시하고자한다.본 연구에 사용된 분류틀은 우종옥 등이 제시한 분석틀을 기초로 하여, 본 연구 목적에 합당하게 재수정하여 사용하였다.

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코티칭 과정에서의 멘토링이 초임 교사의 과학영재교육 관련 PCK 발달에 미치는 영향

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이 연구에서는 사례연구를 통해 멘토링을 통한 코티칭이 초임 과학영재교육 담당교사의 수업 전문성에 미치는 영향을 PCK 측면에서 심층적으로 조사했다. 초임 중등 과학영재교육 담당교사 2 인이 총 4 차에 걸쳐 12 차시의 과학영재수업을 공동으로 계획, 진행, 평가했으며, 2～4 차 수업에서는 수업 전, 중, 후에 멘토링을 실시했다. 두 교사의 수업 계획 과정에 대한 다양한 자료를 수집했고, 모든 수업을 촬영하고 관찰노트를 작성했으며, 모든 면담 내용과 멘토링의 전 과정을 녹음하여 지속적 비교 방법을 통해 분석했다. 연구 결과, 멘토링을 통한 코티칭 과학영재수업 경험이 초임 교사들의 PCK 향상에 효과적이었다. 또한, 코티칭과 멘토링의 결합이 각 전략의 단점을 보완함으로써 긍정적인 상승효과를 일으킬 수 있는 것으로 나타났다. 교사들은 과학영재학생의 다양한 인지적?정의적 특성 계발에 중점을 둔 심화학습을 중심으로 교육과정을 구성하는 것에 대한 확고한 실천적 지식을 갖게 되었으며, 과학영재학생의 다양한 특성과 그에 적합한 교수전략에 관한 지식이 심화되었다. 또한, 과학영재교육 평가의 영역과 방법에 관한 실천적 지식에 향상이 있었으며, 효과적인 탐구학습 지도를 위해 필요한 과학내용지식 측면에도 실질적인 향상이 있었다.

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발표종류: 포스터, 발표일시: 수 16:00~19:00

멘토링을 통한 코티칭 과학영재수업 과정에 대한 초임 교사들의 반성 연구

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이 연구에서는 사례연구를 통해 멘토링을 통한 코티칭 과학영재수업에 대한 중등 초임 과학영재교육 담당교사의 반성의 특징을 생산적 관점에서 조사했다. 중등 과학영재교육 경력이 1 년 미만인 초임 교사 2 인을 선정하여 총 4 회에 걸친 12 차시의 과학영재수업을 공동으로 계획, 진행, 평가하도록 했으며, 2～4 차 수업에서는 수업 전, 중, 후에 멘토링을 실시했다. 두 교사의 모든 코티칭 과학영재수업과 멘토링 과정을 참관했고, 두 교사의 반성일지를 생산적 반성의 관점에서 분석했다. 연구 결과, 수업 차수에 관계없이 두 교사 모두 다른 측면보다 '과학영재 교수전략 및 지도'와 '과학영재학생' 측면에서의 반성을 비교적 많이 하는 것으로 나타났다. 두 측면보다 적긴 했지만 '과학영재교육과정' 측면에 대한 반성도 적지 않았다. '과학내용지식'과 '과학영재교육 평가' 측면에 대한 반성은 드물었다. 통합 수준에 대한 결과에서는, 두 교사 모두 수업의 5 가지 측면 중 2～4 가지 측면이 다양한 형태로 통합된 반성을 하는 것으로 나타났다. 특히 2 가지 측면 간의 통합보다 3～4 가지 측면 간의 통합이 더 많았다. 또한, '과학영재학생' 또는 '과학영재 교수전략 및 지도' 측면이 다른 측면과 통합되어 있는 경우가 많았다. 이런 결과는 멘토링을 통한 코티칭이 초임 과학영재교육 담당교사의 과학 수업에 대한 생산적 반성을 촉진할 가능성을 시사한다.

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2009 개정 교육과정에 의한 중학교 과학 교과서의 삽화에 제시된 성역할 고정관념에 대한 분석

양찬호 박재성 김유진 노태희*

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이 연구에서는 2009 개정 교육과정에 의한 중학교 과학 교과서 27 권에 제시된 삽화에 나타난 성역할 고정관념을 분석하고, 2007 년 개정 교육과정에서의 과학 교과서 분석 결과와 비교하였다. 2009 개정 교육과정에 의한 교과서에서는 모든 학년에서 남학생의 등장 빈도가 여학생보다 높았으며, 이전 교육과정에 의한 교과서에 비해 삽화에 제시된 학생의 성별 등장 빈도 차이가 약간 증가하였다. 특히, 학습외 활동에서는 이전 교육과정에 의한 교과서와 마찬가지로 출판사에 관계없이 성별 등장 빈도의 차이가 컸다. 성인이 제시된 삽화의 경우, 남성의 등장 비율이 여성보다 높았으며 학생 등장 삽화에 비해 성별 간의 차이가 매우 큰 것으로 나타나, 이전 교육과정에 의한 교과서에 비해 별다른 개선이 이루어지지 않았다. 모든 출판사의 교과서에서 가정 활동에서는 여성이, 가정외 활동에서는 남성이 많이 등장하였고, 가정외 활동에서의 차이는 이전 교육과정에 의한 교과서보다 증가하였다. 또한, 대부분의 직업에서 남성의 비율이 높았으며, 교과서에 제시된 과학자는 대부분 남성이었다.

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과학교사 수업 전문성 향상을 위한 협력적 멘토링 과정에서 나타나는 멘토교사의 어려움

최소정 이동원* 남정희

부산대학교 화학교육과

교육의 질적인 향상과 교사의 전문성은 깊은 관계가 있다. 멘토링은 교사 전문성의 향상을 위한 방법이 될 수 있다. 그러나 교사들에게 멘토링에 참여할 기회를 주는 것만으로는 그 효과를 담보하기 어려우며, 멘토링의 질은 멘토의 질에 크게 영향을 받는다. 교사로서 학생들을 가르치는 것과 멘토로서 멘티를 지원하는 것은 다른 맥락이기 때문에 경력이 많은 교사라 하더라도 멘토교사로서 멘티교사를 지도하는 것에는 어려움이 있을 수 있다. 멘토교사 또한 멘토링에 대한 지원이 필요하며 이를 위해서는 먼저 멘토교사가 멘토링에서 어떠한 어려움을 겪는지를 알아볼 필요가 있다. 따라서 이 연구에서는 과학교사 수업 전문성 향상을 위한 협력적 멘토링 과정에서 나타나는 멘토교사의 어려움을 알아보는 것을 목적으로 한다. 이 연구는 1 년 동안 협력적 멘토링에 멘토교사로써 참여한 중등과학교사 7 명을 대상으로 하였으며, 멘토링 과정에서 겪는 멘토교사의 어려움을 알아보기 위해 멘토교사와 멘티교사가 참여한 멘토링 대화, 인터뷰, 설문지, 협의회 등을 분석하였다. 연구 결과, 멘토교사들은 멘토링 초반에 멘토링 범위 설정의 어려움, 멘토로서의 자신감 부족 등을 공통적으로 나타내었으며, 교과나 학교급이 다른 멘토-멘티 쌍의 멘토교사들은 멘티교사의 수업 분석에 어려움을 호소하였다. 하지만 사후 인터뷰 및 설문지 분석 결과 멘토링이 거듭 됨에 따라 멘토교사의 수업 분석 능력과 멘토링 진행 기술이 향상되었으며 멘티교사의 수업 실행 능력 향상에 따라 멘토교사의 자신감이 상승하는 것을 확인할 수 있었다.

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과산화수소 증기를 이용한 유사화학작용제의 제독

김윤기

삼양화학공업(주) 분석기기연구소

과산화수소 증기는 기존 염소계열의 멸균제에 비해 부식성이 낮아 제약 및 의료 분야의 실내멸균제로 사용되며, 암모니아 가스 추가 시 화학작용제의 제독성능이 있다고 알려져 있다. 본 연구에서는 과산화수소 증기를 이용하여 HD, GD, VX 의 유사작용제인 CEPS, DFP, dimethoate 등에 대한 제독효율을 확인하였다. 이를 위해 자체 구성한 과산화수소 기화장치에서 발생시킨 증기를 제독챔버에 주입하여 반응시간을 유지하였다. 제독 후 잔류물을 GC/MS 로 분석한 후 제독효율을 계산하였고, 각각의 유사작용제에 대한 반응 생성물을 통해서 화학작용제의 반응 메카니즘과 유사함을 확인하였다. 실험결과 CEPS 는 30%의 상대습도에서 60 분의 반응시간에 완전제독 되었고, 암모니아 가스 주입의 동반 하에서 DFP 는 30 분, dimethoate 는 150 분의 반응시간에 완전제독 되었다.

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Enhancement of root elongation by iron nanoparticles: Cell wall loosening of plants

신은수 장윤석*

포항공과대학교 환경공학부

The cell wall is a unique feature of plants, not found in animals, and cell wall loosening is essential for plant growth. OH radical-induced cell wall loosening is the only non-enzymatic reaction that degrades matrix polysaccharides in the cell wall. Although reactions mediated by enzymes, including expansin and endo-(1,4)-β-D-glucanase, are well understood, little is yet known about OH radical-induced cell wall loosening. This study showed nano zero-valent iron (nZVI)-derived OH radical-induced cell wall loosening, whereby root length was increased. The oxidation capacity of nZVI, leading to release of H2O2, allowed it to cause OH radical-induced cell wall loosening in roots. The profiles of degraded pectin-polysaccharides in roots were direct evidence for the cell wall loosening. Rapid root elongation led to the reduction of cell wall thickness and resulted in a bias when the cellulose microfibrils were oriented in cell wall. The asymmetrical distribution of tensile strength due to the OH radical-induced cell wall loosening decreased the mechanical strain on the cell walls' girth and enhanced endocytosis. These findings emphasize that OH radical-induced cell wall loosening is important for mechanical regulation of the cell wall and provide new insights into the cellular responses of plants exposed to reactive metal nano-particles.

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Time Trend of PBDEs in Serum Obtained from Korean General Population

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The present study aimed to provide time trend of polybrominated diphenyl ethers (PBDE) in serum obtained from Korean general popualation. The concentration of 7 PBDE congeners (BDE-28, 47, 99, 100, 153, 154, and 183) was determined with 103 human serum collected at 2006. The concentrations of ∑PBDEs (sum of seven congeners) ranged from 0.13 to 31.8 ng g-1 lipid with the median ∑PBDEs concentration of 6.70 ng g-1 lipid. The correlation of PBDE congeners with demographic characteristics and organochlorine contaminants were examined. Based on results of this study and literature, the peak and schematic time trend of ∑PBDEs concentration was estimated. The concentration of ∑PBDEs decreased with time and the peak of ∑PBDEs was before 2001. Furthermore, 6 pooled serum samples covered from 2006 to 2013 were analyzed to observe temporal trend. The highest concentration of ∑PBDEs was shown in 2006 (5.98 ng/g lipid) followed by a decrease in 2013 (2.98 ng/g lipid). Each congener showed different decreasing rates of the concentration.

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Polybrominated Diphenyl Ethers in Korean foods: effect of cooking processes

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Polybrominated diphenyl ethers (PBDEs) are anthropogenic chemicals that have been used in a wide range of consumer products including textiles, electronic equipment, construction materials and flexible foam as addictive flame retardants. Since the first introduction into the market in 1970s, three commercial mixtures of PBDEs have been produced: Penta-BDE, Octa-BDE and Deca-BDE and they were among the most widely used brominated flame retardants (BFRs).When these synthetic compounds enter environmental compartments they could stay there for a long time, sometime up to many years (ref). Persistence and fat-solubility enable PBDEs to bioconcentrate in living bodies and biomagnify along the food chain. Therefore it is important to evaluate the levels of PBDEs in foods as well as dietary exposure of human to these contaminants.We analyzed more than 30 food types on a market-base sampling strategy. All of the samples analyzed were contaminated by PBDEs albeit different levels. BDE-47, 99 and 153 were detected in almost all samples with different weighting ratio depending on the matrix composition whereas BDE-154, 206 and 207 were significant in some meat, fish and shellfish samples. In general, lipid-rich foods often showed higher content of PBDEs in comparison with other type of food. Base on the lipid content we divided food samples into two category: vegetable-based food and lipid-rich food. In both group most of raw foods showed a higher concentration of PBDEs than boiled ones. The losses of PBDEs in boiled samples might either result from thermal degradation, volatilization or increase of water percentage. On the contrary, fried samples showed opposite trends between two categories. Whilst fried plant-based foods had similar or lower PBDE content than starting ingredients, fresh lipid-rich foods contained significant smaller amount of PBDEs when being fried.In conclusion, cooking processes had certain effects on the fate of PBDEs in food. These effects largely depends on the nature of food items. More extensively research would be needed in the future to fully understand the fate of PBDEs through cooking processes.

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Risk Assessments of Polychlorinated biphenyls through Total Diet Study

신은수 장윤석[*]

포항공과대학교 환경공학부

Human exposure of PCBs (Polychlorinated biphenyls) from feed was investigated through TDS (Total Diet Study) for the first time in Korea. Unlike regulatory monitoring for concerned chemicals, TDS is the practical risk assessment aimed at not only raw materials but cooked food samples. Because the concentration of chemicals like PCBs in foods can change during various cooking processes, the risk assessment through TDS using cooked foods is more closer to actual consumed diet. For increasing of representativeness, KNHANES data for 4 years (2008-2011), about 0.07% of Korea population, were combined into a data set. In this study, risk assessment for total PCBs(62 congeners) including DL-PCBs and indicator PCBs was implemented using systematic and continuous TDS approach based on a large-scale data with representativeness and reliability. Average estimation of dietary exposure(6.04 ng/kg b.w./day) through food intake were 30.2% of WHO regulations. When assessments was applied for maximum intaker(95th percentiles), average PCBs intake was 14.88 ng/kg b.w./day, about 74.4% of TDI(20 ng/kg b.w./day). Among the food groups, beverages and liquors(19.8%) and cereals(18.4%) were relatively higher in the contributions of total PCBs. In case of DL-PCBs, average PCBs intake per day per man for Korean populations was 0.09 ng/kg b.w./day, about 2.25~9.00% of TDI(1~4 ng/kg b.w./day) set by WHO. The measurement uncertainty were calculated with multilateral consideration about causable error during proposed analytical procedure of PCBs. The concentration expressions including uncertainty(95% confidence, k=2) toward total PCBs and DL-PCBs are ±11.2188 pg/g, ±1.3658 pg-TEQ/g, respectively.

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Handling Non-detect Data in Environmental Datasets by Using the Kaplan-Meier Method (A Case Study of PCDD/Fs and dl-PCBs in Fish Species)

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포항공과대학교 환경공학부

Many studies were carried out to examine substitution method for handling nondetects in environmental datasets. Some of these studies confirmed that substitution is not a suitable method to deal with nondetects and caused bias. EPA has introduced 3 more intensive statistical methods (Kaplan-Meier, Maximum Likelihood Estimation, and Robust Regression on Order Statistics) for handling nondetects. In this study we examined Kaplan-Meier method for handling nondetet data in PCDD/F and DL-PCB concentration datasets obtained from 240 fish samples collected in Korea in 2012. The method was conducted by ProUCL 4.1 software for environmental applications, downloaded from US-EPA website. The 17 most toxic congeners of PCDD/Fs and 12 dioxin-like PCBs were targeted for analysis. The mean concentration of PCDD/Fs and DL-PCBs obtained by Kaplan-Meier method were 5.72 pg/g ww and 397.34 pg/g ww respectively. Also, the total TEQ concentration (PCDD/Fs+DL-PCBs) among 36 fish species ranged from 0.08 pg WHO-TEQ/g ww (Alaska Pollock and Tuna) to 1.99 pg WHO-TEQ/g ww (Gizzard shad) and no fish sample exceeded the maximum permissible level (6.5 pg WHO-TEQ/g ww). Comparing KM and substitution results in sample approach demonstrated that KM results were slightly higher than substitution results when nondetects were assumed as zero. Also in congener approach, results were near or equal to substitution results when nondetects were assumed equal to LOD. Using the Kaplan-Meier method for calculating the sum and average of datasets including nondetects, leads to easier comparison among the results of different studies. This method avoids the pitfalls of substitution and should be more widely used in statistical analysis of environmental data.

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The exposure assessment of new POPs in multimedia and development of monitoring technology for POPs alternatives

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포항공과대학교 환경공학부

Brominated flame retardants (BFRs) and perfluorinated compounds (PFCs) which have been registered as new persistent organic pollutants (POPs) in Stockholm Convention are considered hazardous substances for human health. These are mainly present in everyday life in the form of daily supplies and the indoor environment rather than the special circumstances occurred in the industrial area. Although the substances are closely related to daily life, there are no researches that the basic information and assessment techniques about integrated human exposure for new POPs and alternate materials. The object of this research was to develop emission assessment techniques, exposure assessment techniques and ecological toxicity assessment. Ultimately, the methods will be applied to develop the integrated human exposure assessment model. On the basis of this research, we are able to reduce the effect of the substances on human body and environment by suggesting reduction and management methods of emission, exposure of new POPs and alternate material and contribute the national strategy for Stockholm Convention.

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Levels and Distribution Characteristics of Hexabromocyclododecane (HBCD) Diastereoisomers in Marine Vertebrates and Invertebrates

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포항공과대학교 환경공학부

Hexabromocyclododecane (HBCD) is a brominated flame retardant extensively used all over the world for expanded and extruded polystyrene (EPS/XPS) insulation applications in buildings and construction industry followed by TBBPA (tetrabromobisphenol A). Three major diastereoisomers (α, β, and γ-HBCD) of HBCD have different characteristics in abiotic and biotic samples, such as sediment, breast milk, fish, and human serum. In the technical mixtures, γ-HBCD is the most preponderant isomer (81.01%) in comparison with α (10.28%), β (8.72%), δ-, and ε-HBCD. Marine vertebrates and invertebrates (i.e., fish and shellfish) have been widely used as typical environmental indicators by showing bioaccumulation of pollutants according to the trophic levels. Additionally, diverse biotransformation enzymes involved in xenobiotics metabolism among different species have demonstrated biotransformation or bioinactivation of xenobiotics. For this reason, distribution characteristics of hexabromocyclododecane (HBCD) in the marine species might substantiate viscerogenic bioisomerization from γ- to α-HBCD and isomerselective uptake of each diastereoisomer, depending on the species with different biotransformation enzymes. In this study, 20 different species of marine invertebrates and 4 different species of marine and freshwater vertebrates were investigated to show the difference of levels and distribution characteristics of HBCD diastereoisomers.

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Characteristics of recovered ITO powder from target waste

최동철 손용근*

성균관대학교 화학과

In this study, our interests were focused on the recovery of ITO from the target waste residue in sputtering chamber. The reason is that ITO target is usually sputtered onto glass plate by DC magnetron sputtering method. Less than 30% of the original target is used for ITO coating on the substrate and the rest of the target would be remain in the chamber. We have prepared ITO powder from the waste for recycling purpose by using co-precipitation method. Waste ITO target powder was dissolved in HCl and then ammonia solution was added to make the InSnOH. After heat treatment up to 400℃ for 6hr, it remained as homogeneous and polycrystalline ITO. The recovered ITO is about 20nm in diameter and appeared as aggregate. XRD pattern of after heat treatment was quite similar to ITO target waste powder. This work was supported the Energy & Resource Recycling of the Korea Institute of Energy Technology Evaluation and Planning (KETEP) grant funded by the Korea government Ministry of Trade Industry and Energy (No.2010501010002B)

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Quantitative detection of carbon nanotube from the mixture of the CNT and graphene using a SYBR green quenching method

정준회 홍인석*

공주대학교 화학과

The present work demonstrates the highly sensitive and selective detection of CNT in water and soil mixture by using biotin-single strand DNA and SYBR green. The various types of CNT (SWNT, MWNTs) were selectively wrapped by single stand biotin tagged DNA, and then wrapped CNTs were selectively isolated by stereptavidin-magnetic beads. Subsequently, isolated CNTs were quantified by SYBR green binding assay. The extent of fluorescence quenching of SYBR green was well correlated to the amount of CNT wrapped by biotin-single strand DNA. The detection limit of this method varies from 10 to 20 ng with respect to different types CNTs.

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The importance of composing natural organic matter in the control of Hg(II) reduction rate by *Shewanella oneidensis* MR-1

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광주과학기술원(GIST) 환경공학부

We examined how microbial Hg(II) reduction in dark and anoxic sediment is affected by the presence of natural organic matter (NOM). For the initial test, we determined Hg(II) reduction rate in the presence of 10 nM Hg(II), 200 μM Elliott soil humic acid (ESHA) as a NOM derivative, and *Shewanella oneidensis* MR-1 in a basal medium as Hg(II)-reducing bacteria. The rate constant of Hg(II) reduction by *Shewanella oneidensis* MR-1 in the presence of ESHA (0.024 ± 0.002 h^{-1}) was higher than that in the absence of ESHA (0.012 ± 0.002 h^{-1}). It appeared that in the presence of ESHA, cells continuously provided electrons to humic acid, which subsequently transferred electrons to Hg(II). The electron transfer from humic acid to Hg(II) has been reported to be relatively fast (3.36 ± 0.79 h^{-1}; Zheng et al., 2012), meaning that the rate of Hg(II) reduction mediated by NOM electron shuttling might be determined by the electron transfer rate from cells to humic acid. The extent of Hg(II) reduction by *Shewanella oneidensis* MR-1 was significantly and positively correlated with organic radical (R^2 = 0.95, linear regression) and aromatic carbon content (R^2 = 0.91, linear regression) in NOM when a variety of NOMs (Anthraquinone-2,6-disulfonate, Suwannee River humic acid, Suwannee River fulvic acid, Pahokee peat humic acid, and Elliott soil humic acid) were tested. Organic radical structures like semi-quinone may play a key role in the transfer of electrons from cells to humic acid. On the whole, the composition of organic matter may significantly affect Hg(II) reduction rate, which poses important implications to the control of Hg(II) bioavailability to Hg(II)-methylating bacteria in natural sediment.

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Effect of metal ratios on catalytic nitrate reduction by Pd-Cu bimetallic catalyst supported by NZVI during continuous batch experiments

HAMIDSHANAWAR 정성윤[1] 배성준[1] 이우진[1,*]

한국과학기술원(KAIST) 건설및환경공학과 [1]*한국과학기술원(KAIST) 건설 및 환경공학과*

Catalytic nitrate reduction by Pd-Cu bimetallic catalyst supported by nanoscale zero-valent iron (NZVI) (Pd-Cu/NZVI) was investigated in continuous batch reactor system. The catalytic reactivity and durability of Pd-Cu/NZVI was evaluated under different experimental condition using various metal ratios (i.e., Pd and Cu). The fundamental experimental condition was set at 1 h HRT, 50 cc/min H2 flow, 1 g/L catalyst loading, 0 to 2% Pd loading, and 0 to 2% Cu loading. Increase in nitrate removal efficiency was observed as Pd concentration gradually increased from 0 to 2% in Pd-Cu/NZVI catalyst with increase in ammonium production. We observed a volcanic trend of nitrogen gas selectivity with maximum value of 33.48% at 0.5% Pd loading. Increase in Pd loading showed stable and efficient nitrate removal (>99%) during the continuous nitrate treatment in 10 h. Similar trends were observed for increase in Cu concentration from 0 to 2% in Pd-Cu/NZVI catalyst. Increase in Cu loading from 0.5 to 1.5% also increased the nitrogen selectivity from 0 to 33.48% and decreased to 25.79% for 2% Cu.

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Vivianite를 이용한 carbon tetrachloride의 환원성 분해에 대한 실험 및 이론적 연구

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자연상의 토양 광물로 유기염소화합물을 환원성 분해하는 기술은 환경적으로 지속가능한 토양 및 지하수 정화 기술로써 높이 평가 받고있다. 본 연구에서는 vivianite(FeII3(PO4)2*8(H2O), 남철석)를 이용해 CT(Carbon tetrachloride, 사염화탄소, CCl4)를 환원 및 탈염소화 시키는 회분식 실험을 수행하였다. 다양한 환경 인자들 중 CT 의 초기 농도, 현탁액의 pH(pH 5~9), 그리고 주요 경쟁 이온(Ca2+, HCO3-)의 유무가 CT 분해 속도에 큰 영향을 미치는 것으로 나타났다. 더불어 Vivianite 에 의한 CT 분해 기작을 논하기 위해 반응 시간에 따른 부산물들의 농도 변화도 측정하였다. 또한 vivianite 표면에서 일어나는 상호작용을 분자 수준의 미시적 관점에서 이해하기 위하여 양자 계산(QC, Density Functional Theory method, software: Maestro and Cerius 2)을 수행, 결합에너지를 추산하였다. 이러한 결과에 기반하여 CT 의 탈염화 과정에 알맞은 반응 부산물 및 상세한 기작 원리를 이론적으로 설명할 수 있다. 특히 HCCl3 가 vivianite 표면에서 직접적으로 환원되지 않으며, 이는 불안정한 구조(결합에너지 5.178 eV)를 형성하기 때문인 것으로 해석된다. 대신 염소 이온(Cl-)이 수산화이온(OH-) 또는 물과 상호 반응 후 서로 자리를 바꾸기 때문에 주된 중간산물로 HCOOH 를 생성하게 된다. 향후의 실제 환경에서의 CT 분에 공정 설계 및 운용에 본 연구의 실험 및 이론적 결과들을 적용할 수 있을 것이라 전망한다.

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XAFS and QC study for the molecular-scale verification of interaction mechanism between Cr(VI) and vivianite

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Hexavalent chromium (Cr(VI)) is one of the popular toxic heavy-metals and it can be accidentally released from variable sources (mine, metallurgy, electrical device industry) to environment, especially subsurface. Here we have studied interaction mechanism of aqueous Cr(VI) with vivianite (FeII3(PO4)2?8(H2O)) under natural analogue conditions (pH 5-9 and presence of competing ions (Ca2+, HCO3-)). Complete removal of Cr(VI) by vivianite was observed within 1 min. at pH 9. As pH increased, Cr(VI) removal kinetic was decreased following 100% removal in 12 hr at pH 7; 100% removal in 24 hr at pH 9. This phenomena might have resulted from electrostatic interaction between charged vivianite surface (PZCvivianite: 5.3) and major Cr(VI) species (CrO42-, HCrO4-) under the pHs. Geochemical modeling (MINTEQL+) results showed the formation of different Cr(VI) species (CaCrO4, CrO42-) in the presence of competing ions, however, it did not affect the Cr(VI) removal kinetic by vivianite. Quantum Calculations (Maestro and Cerius 2) was used to calculate the binding energies between Cr(VI) species and vivianite surface. The results indicated that Cr and O atom of Cr species are preferred to bind with Fe and O atom of vivinaite surface, respectively. Therefore, regardless of Cr(VI) species type, Cr(VI) can be removed by vivianite via form of Cr-Fe, Cr-O, and O-Fe bindings. EXAFS analysis results have supported our conclusions by shown the similar binding properties (binding distance and angle). The molecular scale investigations using XAFS and QC showed that Cr(VI) bound on the vivianite surface was reduced to Cr(III)-oxide by receiving electrons from Fe(II) of vivianite surface.

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Effect of environmental factors on the reductive dechlorination of tetrachloroethene by nano-mackinawite catalyzed by cobalamin

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We carried out a parametric study on tetrachloroethene (PCE) dechlorination by nano-mackinawite (nFeS) catalyzed with cobalamin (Cbl) to investigate effects of environmental factors on the degradation of PCE by nFeS-Cbl. Selected environmental factors were Cbl type (methylcobalamin (Cbl-CH_4), aquocobalamin (Cbl-OH), and cyanocobalamin(Cbl-CN)), pH, nFeS-Cbl concentration, and different cations and anions. Among three Cbls, Cbl-CN showed the fastest dechlorination kinetics of PCE at pH 8.3 (45% at 120 hr). Kinetic rate constants increased from 0.0017 to 0.1003 hr^{-1} with increasing pH from 5 to 12. When nFeS concentration increased from 0.05 to 5 g, the kinetic rate constants increased from 0.0423 to 0.3557 hr^{-1}. In case of varing Cbl-CN concentrations (0-1.0 mM), dechlorination kinetic rate constant increased to 0.9870 hr^{-1} with the increase of Cbl-CN concentration from 0 to 0.5 mM. However, the kinetic rate constants showed a saturation pattern at higher concentration of the Cbl-CN than 0.5 mM. Effect of cations (Na^+, K^+, Mg^{2+}, and Ca^{2+}) and anions (CO_3^{2-}, SO_4^{2-}, NO_3^-, and HCO_3^-), possible ions easily found in natural groundwater, was investigated. When those ions were added to nFeS-Cbl solution, most ions, except HCO_3^-, showed the accelerated PCE dechlorination kinetics. The results obtained in this study can be used to provide basic knowledge of environmental factors on reductive dechlorination of PCE by biomimetic catalyst and to establish optimal operation condition to treat PCE in groundwater.

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Mussel-inspired adhesive protein-based electrospun nanofibers reinforced by Fe(III)-DOPA complexation

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Marine mussels utilize multiple bidentate complexes formed by Fe(III) and DOPA in mussel adhesive protein (fp-1) to reinforce tough and elastic byssal fibers as a specialized underwater adhesive aid. In this study, mussel-inspired electrospun nanofibers were fabricated using recombinant mussel adhesive protein (rfp-1), Fe(III)-DOPA complexes, and polycaprolactone. The mechanical properties of the fabricated nanofibers were reinforced by the Fe(III)-DOPA complex found in fp-1, which is a key component of the naturally occurring high-performance mussel fiber coating. Experimental results show that the stoichiometry of Fe(III)-DOPA complexes in the nanofibers could be controlled by buffer pH conditions and the stiffness of the nanofiber mat increased linearly with the concentration of the Fe(III)-DOPA complexes, as monitored by resonance Raman spectroscopy. This suggests the potential of Fe(III)-DOPA complexation as an effective strategy for enhancing the mechanical properties of nanofibrous biomedical materials.

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Down-Stream Current Draining Effect of Cadmium Recovery System Using a Double Microbial Fuel Cell Arrangement

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In order to recover cadmium from a cadmium ion-containing artificial wastewater, a double microbial fuel cell (d-MFC) arrangement with each chamber containing 200 mL solution was applied. When powering Cd(II)-MFC for 60 hours by Cr(VI)-MFC, the recovery efficiencies of cadmium ions were 93.43 ± 0.17%, 93.30 ± 0.74%, and 89.73 ± 0.28% for initial concentrations of 50 ppm, 100 ppm, and 200 ppm, respectively. This research represents that by quickly removing electrons generated on the bio-anode by microorganisms to a down-stream drain, a mediator formation could be accelerated by the Le Chatelier’s principle. The drained maximum power density (21 Wm-2) was 10.5 times higher than the power directly supplied to the Cd(II)-MFC.